

**Agilent Technologies MassHunter Quantitation version 12  
Quantitation DataSet Overview**

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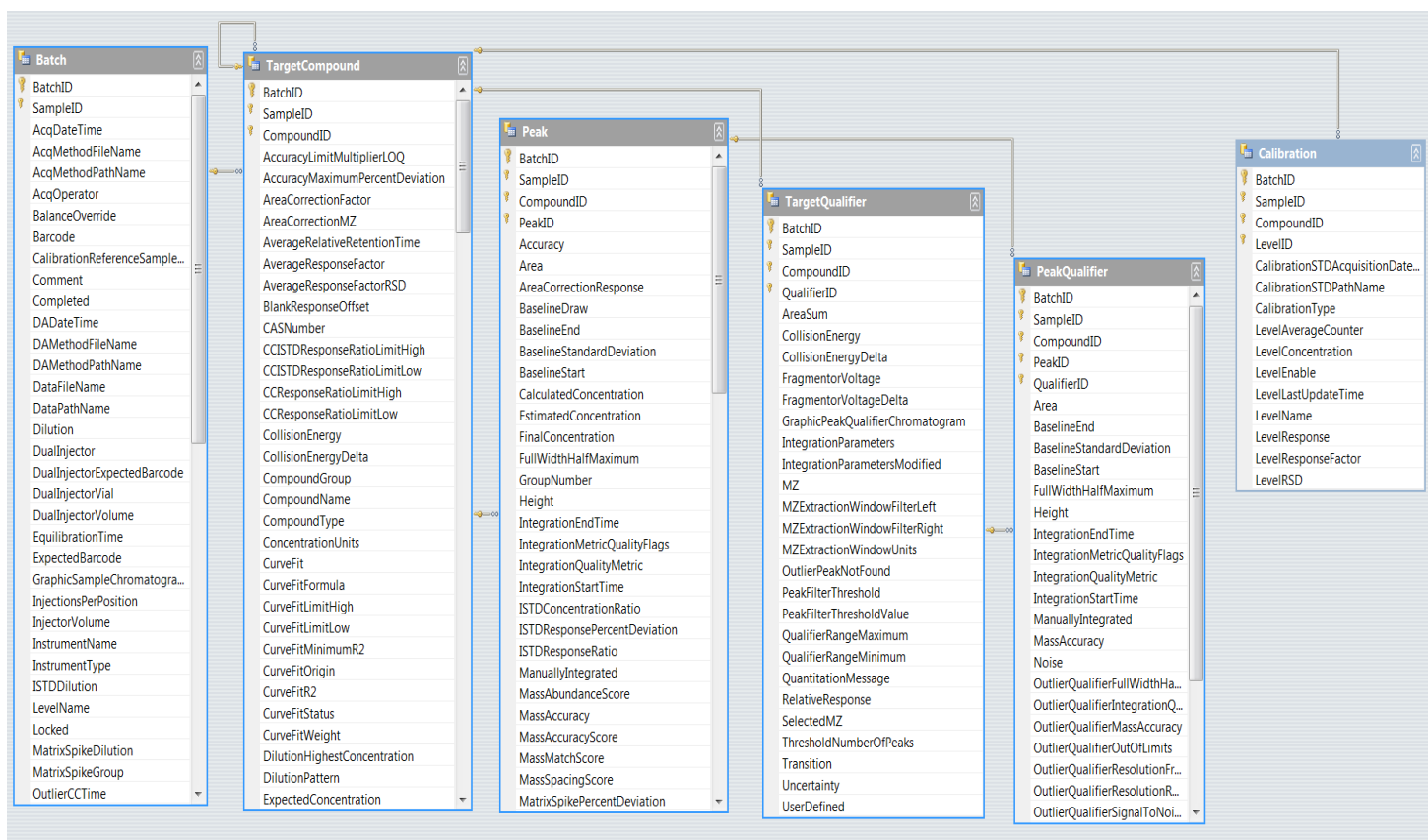
# Quantitation DataSet Overview

The Quantitation DataSet is an in-memory relational database which stores all the quantitation information and the relationships between sample, compound(s), qualifier(s), and calibration. A one to many (1:n) relationship exists between the following tables:

- Each Batch (sample) has one or more TargetCompounds.
- Each TargetCompound (method) has one or more TargetQualifiers (method).
- Each TargetCompound (method) has one or more Peaks (results).
- Each Peak (results) has one or more QualifierPeaks (result).
- Each TargetCompound has one Calibration.

As a general rule, Target tables hold the method, and Peak tables hold the results.

- The TargetCompound and TargetQualifier tables store the method information for the compounds and their qualifiers, respectively.
- The Peak and PeakQualifier tables store the result information for the compounds and their qualifiers, respectively.



# Results

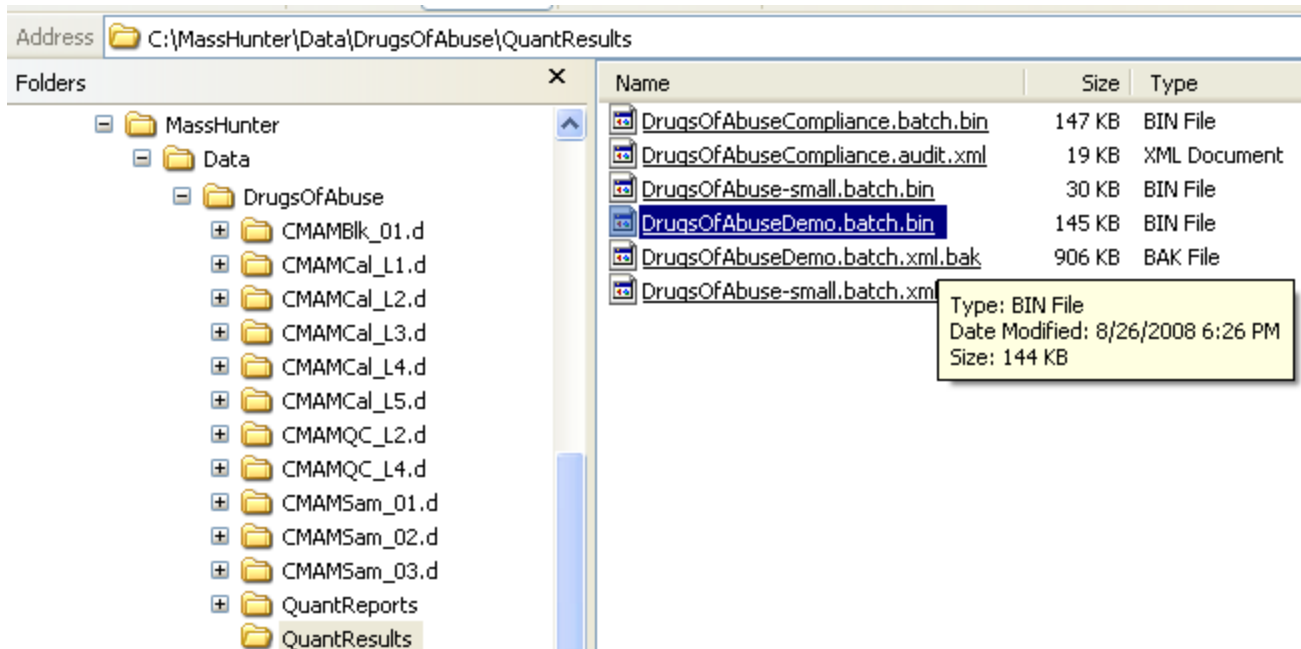
Differentiates analysis and reporting results.

## Analysis

Analysis results are stored in an XML document in a [relational](#) database format.

Analysis results are stored when you save a batch.

Note that only the columns that assigned values are persisted in the results. Column assigned NULL are not persisted in the XML document.



**Results 1:** Analysis results are stored in QuantResults directory.

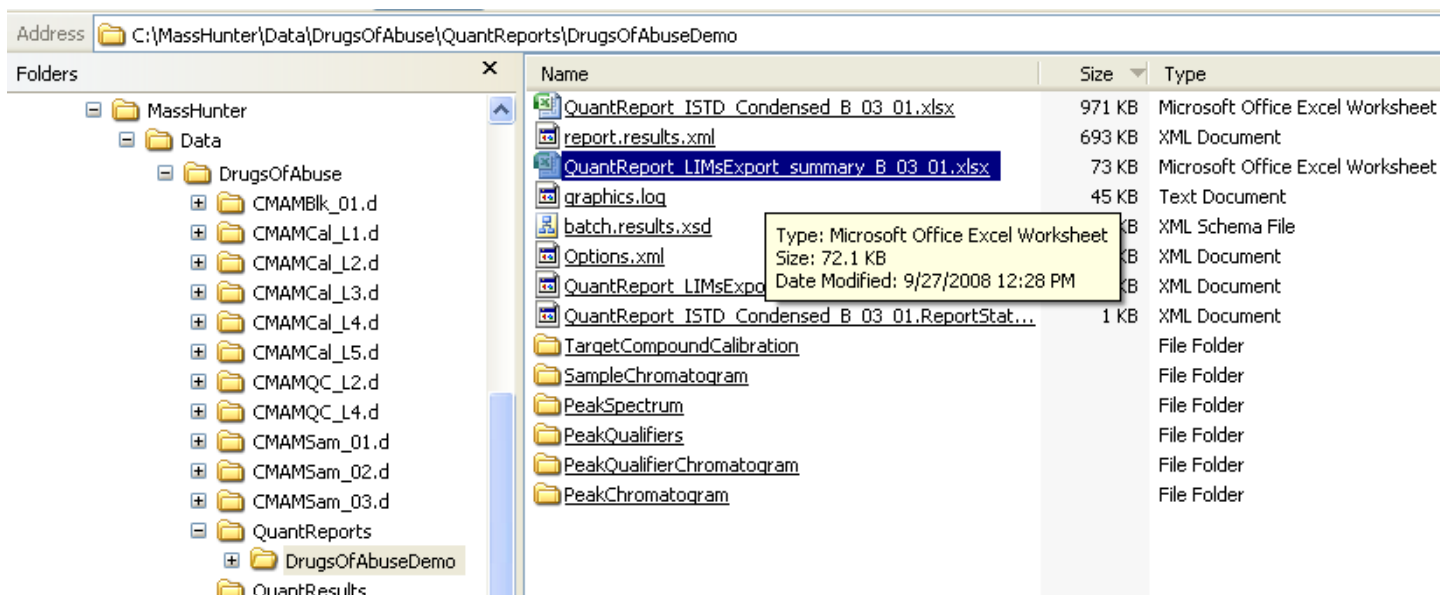
**Note** that the analysis results are stored in DrugsOfAbuseDemo.batch.bin binary file for reasons of size and speed.

# Reporting

Reporting results are stored in an XML document in a [hierarchical](#) database format.

Reporting results are stored when you generate a report. Reporting results are then delivered to the [Excel](#) reporting subsystem.

Reporting results serve as the input to an upload to an external database. Typically, the external database parses out the summary results using XML [XPath](#) technology and maps those results into the customers existing database.



**Results 2: Reporting results stored in QuantReports directory under the BatchName.**

**Note the Excel 2007 workbook as QuantReport\_LIMsExport\_summary\_B\_03\_01.xlsx**

**Note the results XML document as report.results.xml**

**Note the directories which contain the graphics files as .emf**

# Globalization

Below are reference tables designed to use XPath expressions to find and replace Enum Names (string values in the reporting results) with UI Names (localized string values in the reporting results). Additional enum-related tables are located with their respective column definitions.

The approach is to translate the reporting results to the local strings. The reporting results are then imported into a localized template producing a localized Excel report. Note that the underlying schema does not change, only the reporting result values.

<b>Enum Name</b>	<b>UI Name</b>	<b>XPath expression</b>
false	false	*//@*[.='true']
true	true	*//@*[.='false']
true	true	*//*[.='true']
false	false	*//*[.='false']
High	High	*//*[.='High']
Low	Low	*//*[.='Low']

<b>Enum Name</b>	<b>UI Name</b>	<b>Example XPath expression</b>
High	High	*//OutlierAccuracy[.='High']
Low	Low	*//OutlierAccuracy[.='Low']

# Relationships

A *one to many* (1:n) relationship exists between the following tables:

Each Batch (sample) has one or more TargetCompounds.

Each TargetCompound (method) has one or more TargetQualifiers (method).

Each TargetCompound (method) has one or more Peaks (results).

Each Peak (results) has one or more QualifierPeaks (result).

Each TargetCompound has one Calibration.

As a general rule, "Target" tables hold the method, and "Peak" tables hold the results.

Specifically,

The TargetCompound and TargetQualifier tables store the method information to the compounds and their qualifiers, respectively.

The Peak and PeakQualifier tables store the result information for the compounds and their qualifiers, respectively.

# Data Types

Below are definitions of the data types used in the Quantitation DataSet.

## Boolean

Boolean represents "True" or "False".

## Double

Double represents a 64 bit floating point number. The number ranges from  $\pm 4.9E-324$  to  $\pm 1.7976931348623157E+308$ .

## Integer

Integer represents a 32 bit signed integer. The number ranges from -2147483648 to 2147483647.

## Short

Integer represent a 16 bit signed integer. The number ranges from -32768 to 32767.

## Byte

Byte represents an 8 bit signed integer. The number ranges from -128 to 127.



## DateTime

Date-Time format follows ISO 8601 XML-compliant representation of dates and times.

All timezoned times are Coordinated Universal Time (UTC, sometimes called "Greenwich Mean Time"). The presentation shows the "Local" or untimezoned times.

### Example:

The Date-Time string 2008-01-20T19:00:00.

## DateTimeOffset

Date-Time Offset represents a point in time, typically expressed as a date and time of day, relative to Coordinated Universal Time (UTC). The DateTimeOffset structure includes a DateTime value, together with an Offset property that defines the difference between the current DateTimeOffset instance's date and time and UTC.

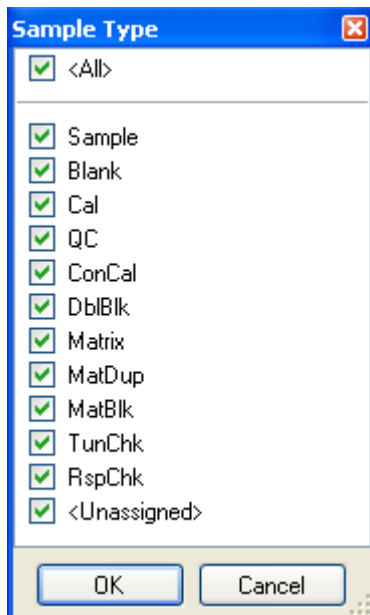
## String

[String](#) represents a set of characters.

String values are often enumerations representing different categories.

### Example:

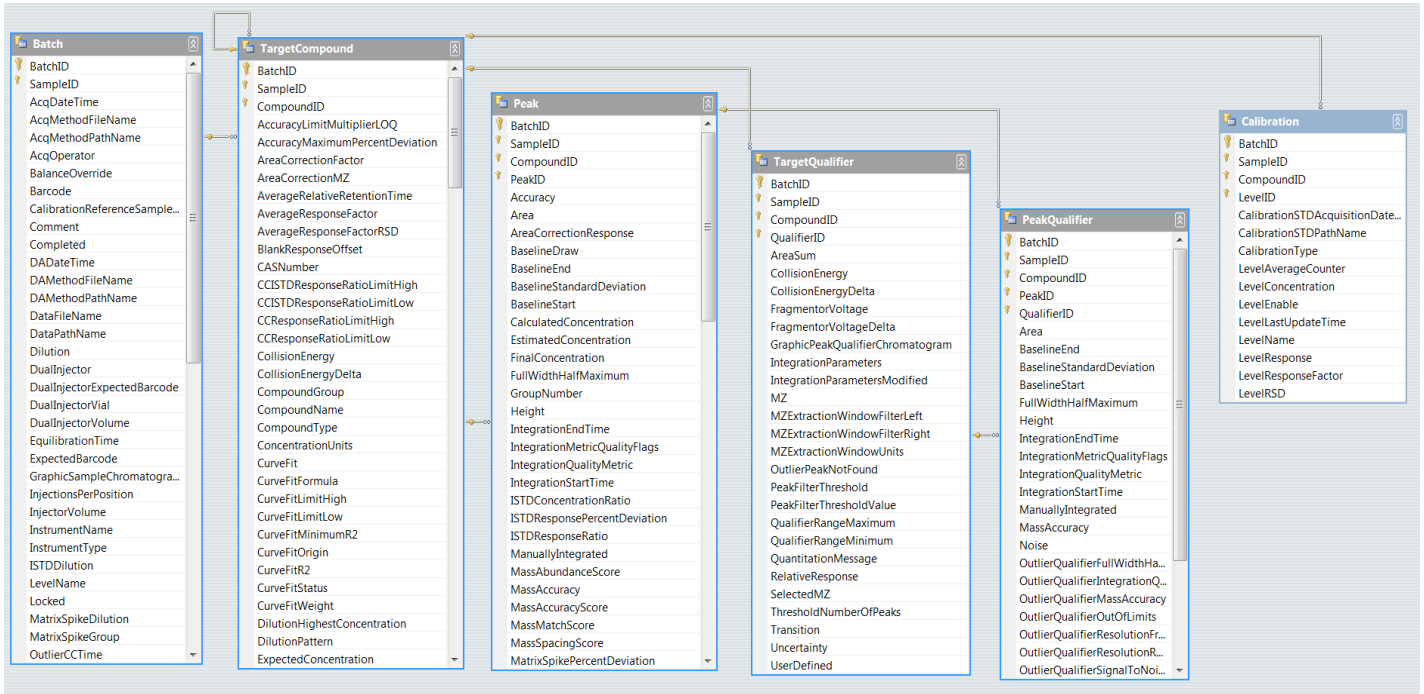
The following set:



Categories: Choices for Sample Type.

# Quantitation DataSet schema

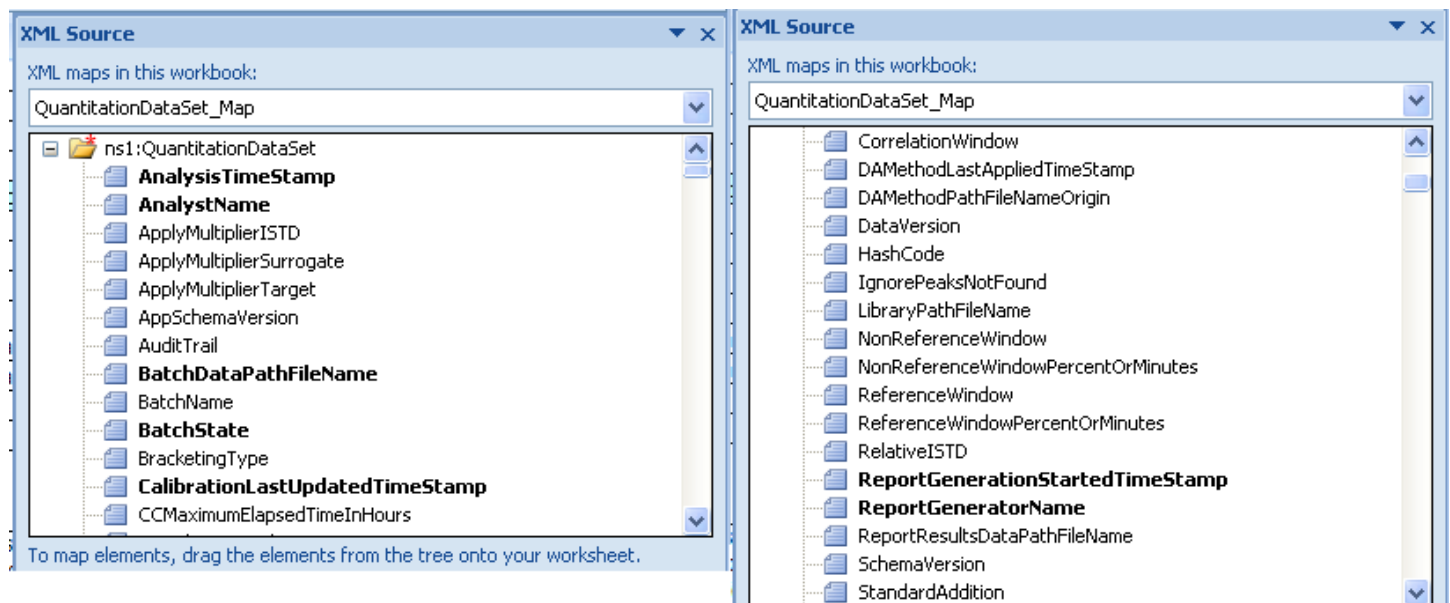
Below are the details of each column ([XML](#) attributes and elements) organized by the hierarchy of tables in the [DataSet](#).



**DataSet 1: The Quantitation DataSet is an in-memory relational database which stores all the quantitation information and the relationships between sample, compound(s), qualifier(s), and calibration.**

# Globals

Below are the definitions of the globals (XML attributes) that pertain to the entire batch.



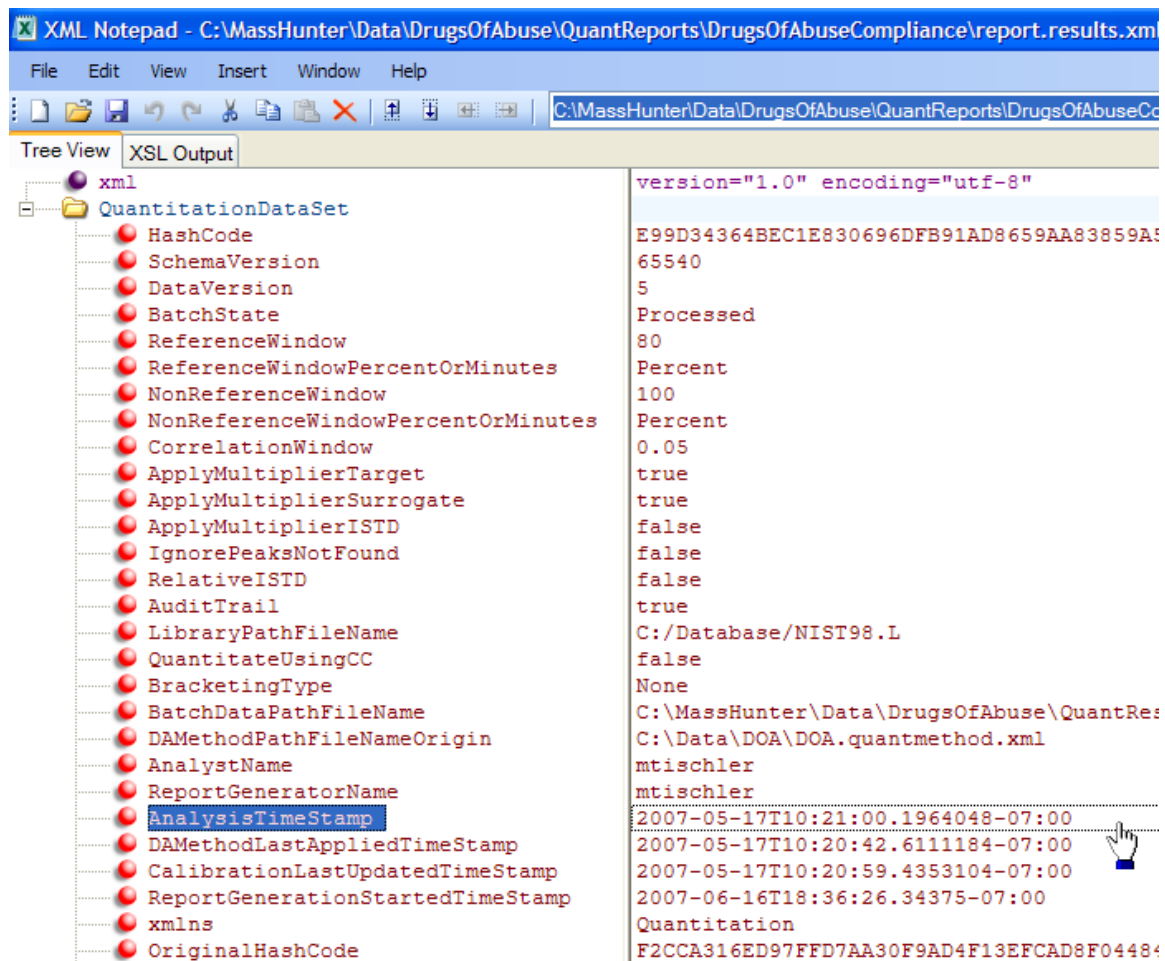
**DataSet 2:** Shows the globals from the [Excel XML mapping](#).

# AnalyzeQuantVersion

[AnalyzeQuantVersion](#) designates the version of Quantitation software when batch is saved.

# AnalysisTimeStamp

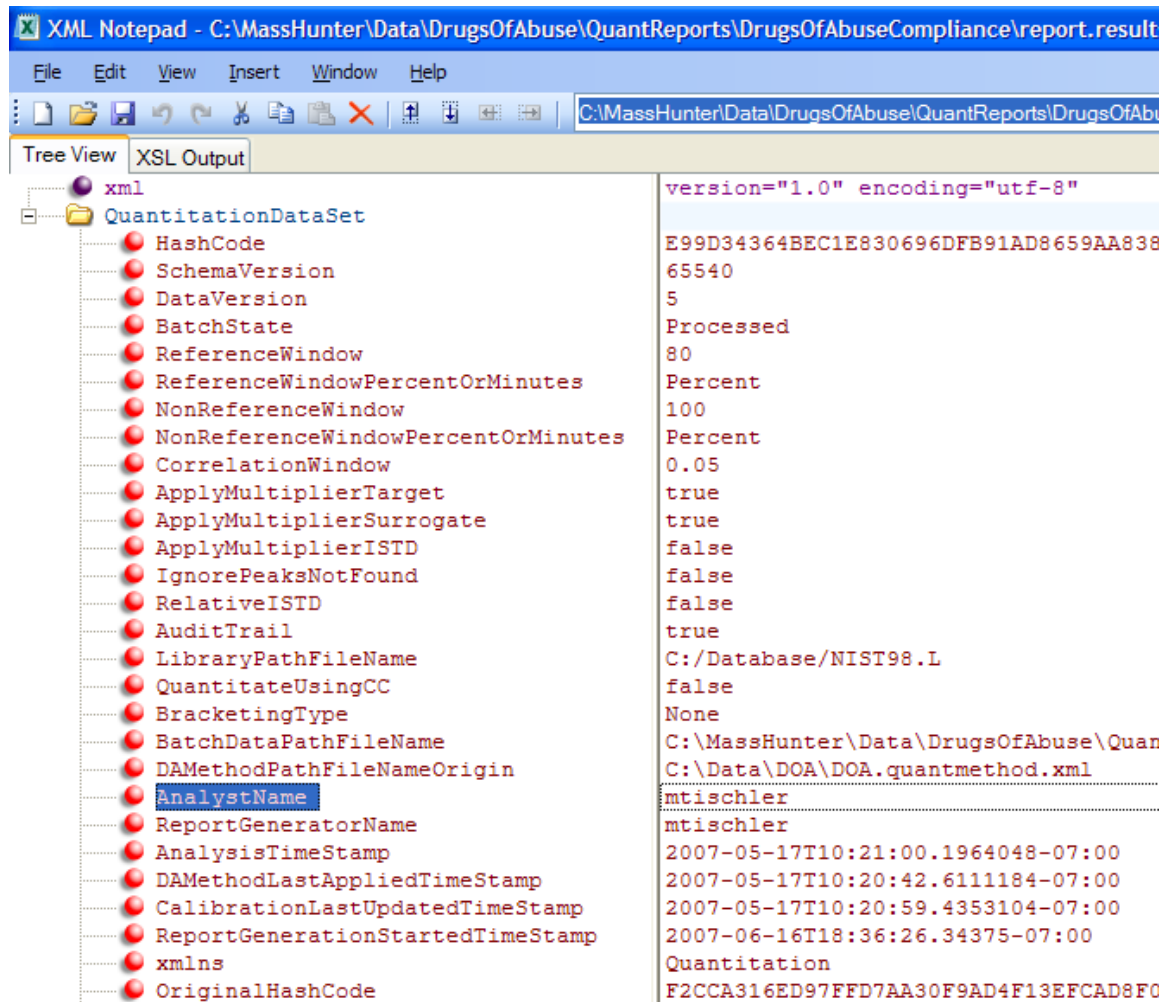
[AnalysisTimeStamp](#) is the date and time for last change to the results. AnalysisTimeStamp is set whenever re-calculation occurs in Batch-at-a-Glance.



**DateTime 1:** Records the datetime in XML format.

# AnalystName

[AnalystName](#) is the name of person logged on who generated these results. The name is fetch from the environment which reflects the user's logon information. AnalystName is set when reports are generated.



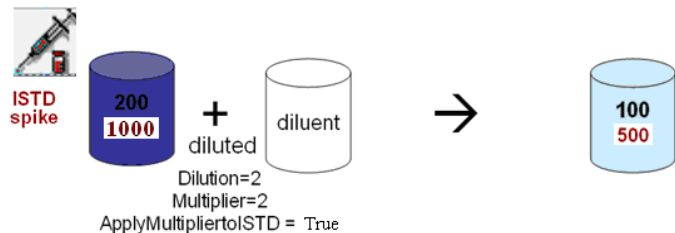
The screenshot shows an XML Notepad window displaying the contents of a file named 'report.result.xml'. The XML structure is shown in a tree view on the left, with the 'AnalystName' field highlighted. The corresponding XML text is shown on the right.

Field Name	Value
version	"1.0" encoding="utf-8"
HashCode	E99D34364BEC1E830696DFB91AD8659AA838
SchemaVersion	65540
DataVersion	5
BatchState	Processed
ReferenceWindow	80
ReferenceWindowPercentOrMinutes	Percent
NonReferenceWindow	100
NonReferenceWindowPercentOrMinutes	Percent
CorrelationWindow	0.05
ApplyMultiplierTarget	true
ApplyMultiplierSurrogate	true
ApplyMultiplierISTD	false
IgnorePeaksNotFound	false
RelativeISTD	false
AuditTrail	true
LibraryPathFileName	C:/Database/NIST98.L
QuantitateUsingCC	false
BracketingType	None
BatchDataPathFileName	C:\MassHunter\Data\DrugsOfAbuse\Quan
DAMethodPathFileNameOrigin	C:\Data\DOA\DOA.quantmethod.xml
<b>AnalystName</b>	<b>mtischler</b>
ReportGeneratorName	mtischler
AnalysisTimeStamp	2007-05-17T10:21:00.1964048-07:00
DAMethodLastAppliedTimeStamp	2007-05-17T10:20:42.6111184-07:00
CalibrationLastUpdatedTimeStamp	2007-05-17T10:20:59.4353104-07:00
ReportGenerationStartedTimeStamp	2007-06-16T18:36:26.34375-07:00
xmlns	Quantitation
OriginalHashCode	F2CCA316ED97FFD7AA30F9AD4F13EFCAD8F0

**Name 1: Records user name.**

## ApplyMultiplierISTD

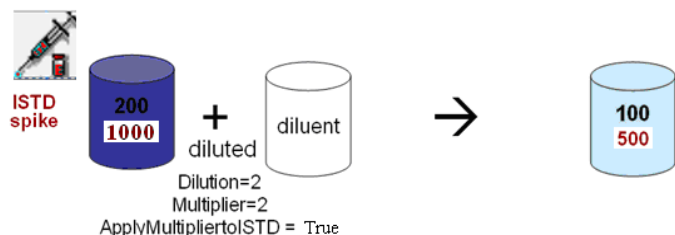
[ApplyMultiplierISTD](#) represents the selection to apply the sample [Multiplier](#). The sample multiplier is a multiplicative operation on the [FinalConcentration](#). A sample multiplier of "2" will double the reported concentration of the affected compound types.



ApplyMultiplierISTD may be useful in adjusting samples that were prepared with different ISTD concentrations.

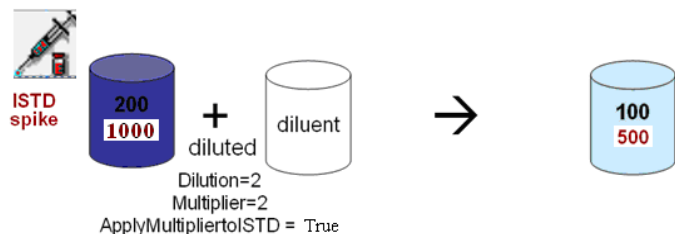
## ApplyMultiplierMatrixSpike

[ApplyMultiplierMatrixSpike](#) represents the selection to apply the sample [Multiplier](#). The sample multiplier is a multiplicative operation on the [FinalConcentration](#). A sample multiplier of "2" will double the reported concentration of the affected compound types.



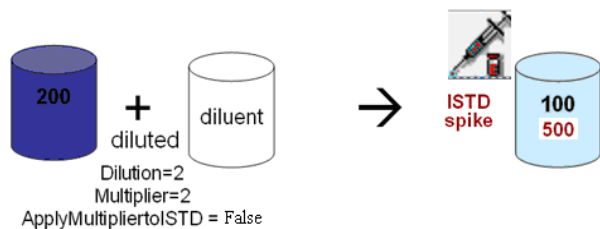
## ApplyMultiplierSurrogate

[ApplyMultiplierSurrogate](#) represents the selection to apply the sample [Multiplier](#). The sample multiplier is a multiplicative operation on the [FinalConcentration](#). A sample multiplier of "2" will double the reported concentration of the affected compound types.



## ApplyMultiplierTarget

[ApplyMultiplierTarget](#) represents the selection to apply the sample [Multiplier](#). The sample multiplier is a multiplicative operation on the [FinalConcentration](#). A sample multiplier of "2" will double the reported concentration of the affected compound types.



## AppSchemaVersion

[AppSchemaVersion](#) designates the Quantitation DataSet schema version used by the currently running Quant application instance.

## AuditTrail

[AuditTrail](#) records the state of audit trail for this batch.



# BatchDataPathFileName

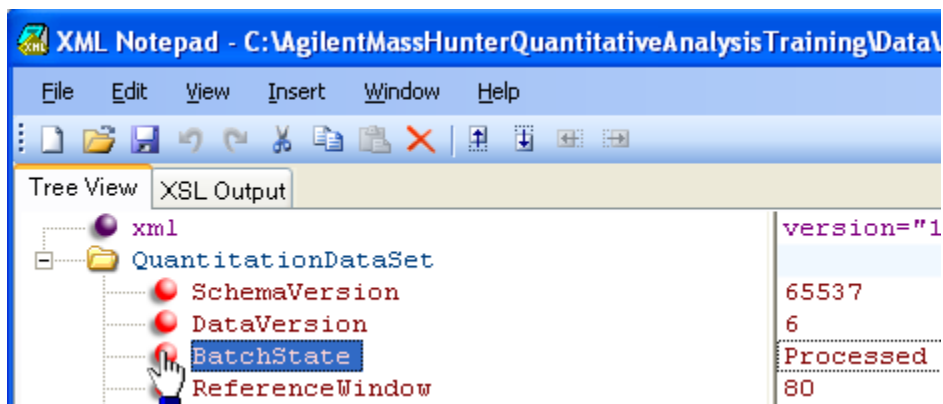
[BatchDataPathFileName](#) is the file system path and file name to the batch analysis results. Saving the batch sets the BatchDataPathFileName.

# BatchName

[BatchName](#) is the user-defined name for the collection of samples analyzed together.

# BatchState

[BatchState](#) is an internal quantitation state that records the synchronization of the analysis.



BatchState 1: "Processed" when analysis completed.

Enum Name	UI Name	XPath expression
Initial	Initial	*//@BatchState[.='Initial']
Processed	Processed	*//@BatchState[.='Processed']
ResultsCleaned	ResultsCleaned	*//@BatchState[.='ResultsCleaned']
ResultsDirty	ResultsDirty	*//@BatchState[.='ResultsDirty']

# BracketingType

[BracketingType](#) changes the association between samples and their calibration samples. The purpose of bracketing is to reduce uncertainty of the calibration curve applied to a particular sample.

By default, all the calibration samples grouped in a batch to create the calibration curve. In other words, the position of the calibration samples with respect to a sample block does not affect the sample's calibration curve. All samples share the same calibration curve regardless.

BracketingType set to Overlapped groups the set of Calibration and QCs above the below a set of samples and averages that group of Calibration and QCs to generate a calibration curve that is applied to those "bracketed" samples. In this manner, the "bracketed" samples receive a calibration curve created from calibration samples whose variation is minimized.

SampleName	SampleType	LevelName	Position	Comment
CAL1	Calibration	L1	1	First calibration block
CAL2	Calibration	L2	2	Use 1 <sup>st</sup> and 2 <sup>nd</sup> cal block averaged
CAL3	Calibration	L3	3	
SAMP1	Sample		11	Calibration using
SAMP2	Sample		12	1 <sup>st</sup> and 2 <sup>nd</sup> cal block averaged
SAMP3	Sample		13	Assign each sample this
SAMP4	Sample		14	Calibration table unique for
SAMP5	Sample		15	This sample block
CAL1	Calibration	L1	1	Second calibration block
CAL2	Calibration	L2	2	Use 1 <sup>st</sup> and 2 <sup>nd</sup> cal block averaged
CAL3	Calibration	L3	3	
SAMP1	Sample		16	Calibration using
SAMP2	Sample		17	2 <sup>nd</sup> and 3 <sup>rd</sup> cal block averaged
SAMP3	Sample		18	Assign each sample this
SAMP4	Sample		19	Calibration table unique for
SAMP5	Sample		20	This sample block
CAL1	Calibration	L1	1	Third calibration block
CAL2	Calibration	L2	2	Use 2 <sup>nd</sup> and 3 <sup>rd</sup> cal block averaged
CAL3	Calibration	L3	3	

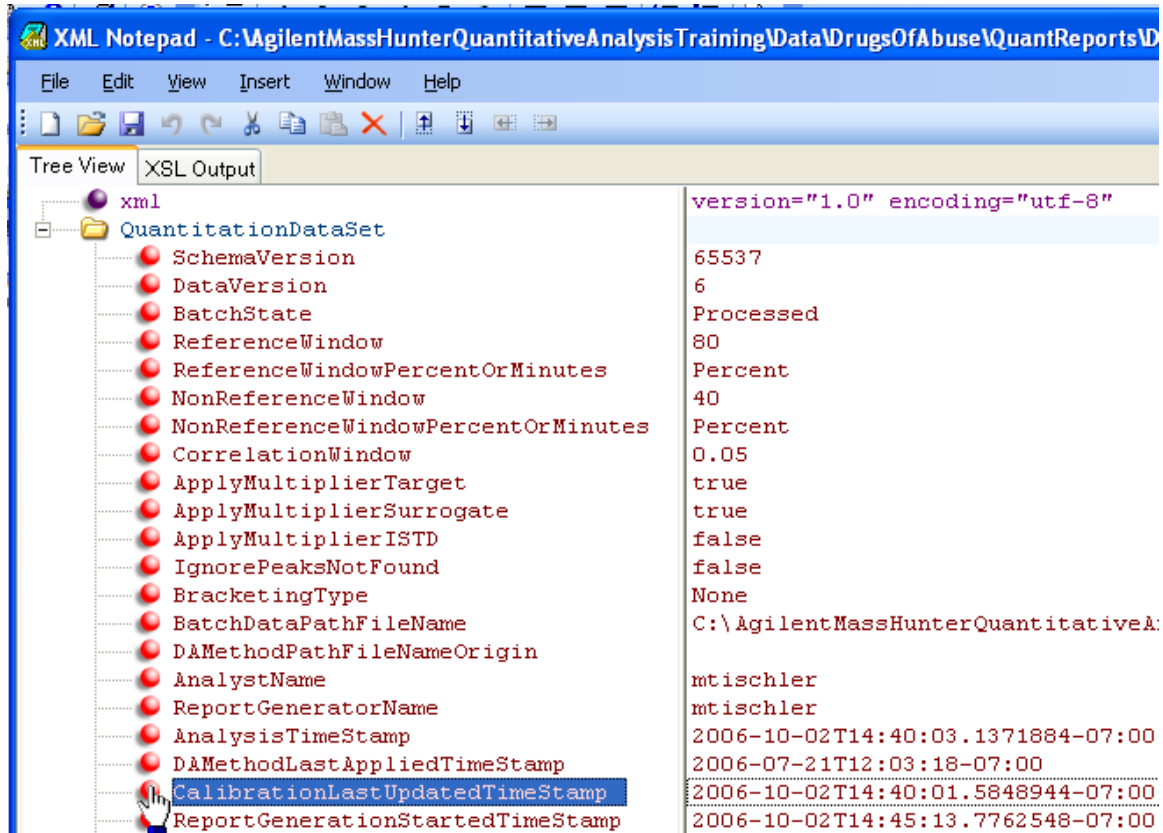
**Bracketing 1:** In this example, the first sample block [Positions 11,12,13,14,15,] use the calibration curve created from the CAL1, CAL2, CAL3 samples above and below that sample block. Similarly, the next sample block [Positions 16,17,18,19,20] uses the CAL1, CAL2, CAL3 (overlapped) above and the CAL1, CAL2, CAL3 sample below. Hence, the name overlapped averaged bracketing.

BracketingType set to "SampleGroup", for each compound in each sample, only the calibration samples that share the same Sample Group attribute as the sample in question are used to compute the compound calibration table.

Enum Name	UI Name	XPath expression
None	None	*//@BracketingType[.='None']
Overlapped	Overlapped	*//@BracketingType[.='Overlapped']
SampleGroup	SampleGroup	*//@BracketingType[.='SampleGroup']

# CalibrationLastUpdatedTimeStamp

[CalibrationLastUpdatedTimeStamp](#) is the date and time for last change to the calibration table. Set whenever the Calibration information is recalculated. For example, re-analyzing the batch re-builds the calibration table that resets this timestamp.



Element Name	Value
version	"1.0" encoding="utf-8"
SchemaVersion	65537
DataVersion	6
BatchState	Processed
ReferenceWindow	80
ReferenceWindowPercentOrMinutes	Percent
NonReferenceWindow	40
NonReferenceWindowPercentOrMinutes	Percent
CorrelationWindow	0.05
ApplyMultiplierTarget	true
ApplyMultiplierSurrogate	true
ApplyMultiplierISTD	false
IgnorePeaksNotFound	false
BracketingType	None
BatchDataPathFileName	C:\AgilentMassHunterQuantitativeA
DAMethodPathFileNameOrigin	
AnalystName	mtischler
ReportGeneratorName	mtischler
AnalysisTimeStamp	2006-10-02T14:40:03.1371884-07:00
DAMethodLastAppliedTimeStamp	2006-07-21T12:03:18-07:00
<b>CalibrationLastUpdatedTimeStamp</b>	<b>2006-10-02T14:40:01.5848944-07:00</b>
ReportGenerationStartedTimeStamp	2006-10-02T14:45:13.7762548-07:00

**DateTime 2: Records DateTime in XML format.**

# CCMaximumElapsedTimeInHours

[CCMaximumElapsedTimeInHours](#) records the maximum allowed difference in time between any sample and the CC sample type in that batch.

# ComplianceName

[ComplianceName](#) records the compliance module name. e.g. ECM.

## ComplianceServer

[ComplianceServer](#) records the server path that contains the batch file.

## ComplianceVersion

[ComplianceVersion](#) records the compliance module version.

# CorrelationWindow

[CorrelationWindow](#) represents the size of the correlation window.

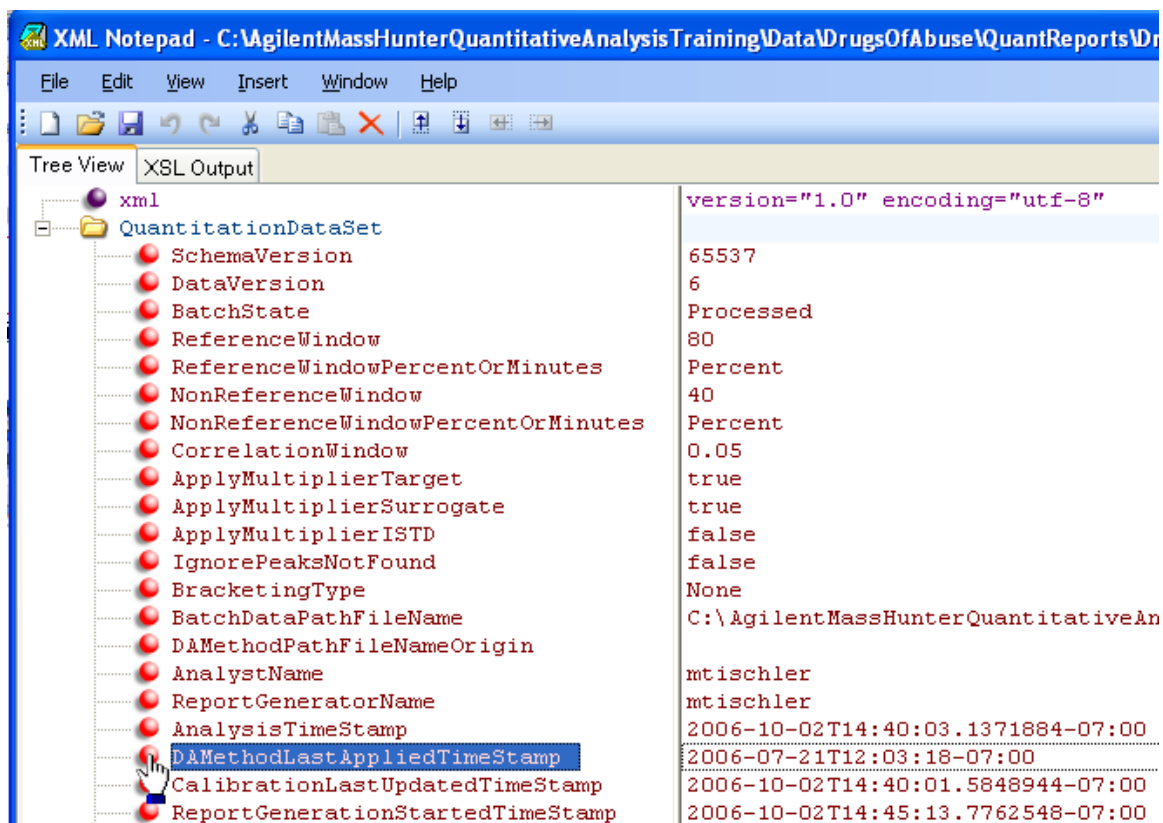
CorrelationWindow is used in processing the current data file to determine if peaks found during integration of the target and qualifier signals are due to the same chromatographic elution (i.e., have the same retention time). The units are minutes.

## Example:

Change the RT correlation window from 1 minute to 2 minutes helps the quantitation algorithm to associate the qualifier peak with the quantifier from same compound.

# DAMethodLastAppliedTimeStamp

[DAMethodLastAppliedTimeStamp](#) records the date and time for last change to the method. Set whenever the method is edited in the Method Editor and then applied to Batch.



Parameter	Value
SchemaVersion	65537
DataVersion	6
BatchState	Processed
ReferenceWindow	80
ReferenceWindowPercentOrMinutes	Percent
NonReferenceWindow	40
NonReferenceWindowPercentOrMinutes	Percent
CorrelationWindow	0.05
ApplyMultiplierTarget	true
ApplyMultiplierSurrogate	true
ApplyMultiplierISTD	false
IgnorePeaksNotFound	false
BracketingType	None
BatchDataPathFileName	C:\AgilentMassHunterQuantitativeAn
DAMethodPathFileNameOrigin	
AnalystName	mtischler
ReportGeneratorName	mtischler
AnalysisTimeStamp	2006-10-02T14:40:03.1371884-07:00
<b>DAMethodLastAppliedTimeStamp</b>	<b>2006-07-21T12:03:18-07:00</b>
CalibrationLastUpdatedTimeStamp	2006-10-02T14:40:01.5848944-07:00
ReportGenerationStartedTimeStamp	2006-10-02T14:45:13.7762548-07:00

**DateTime 3: Records DateTime in XML format.**

**Note that DateTime recorded in XML standard DateTime format.**

# DAMethodPathFileNameOrigin

[DAMethodPathFileNameOrigin](#) designates the path and file name where the method originally was opened and applied. When a user opens a method from an existing file and applies that method to the batch, Batch-at-a-Glance records the DAMethodPathFileNameOrigin.

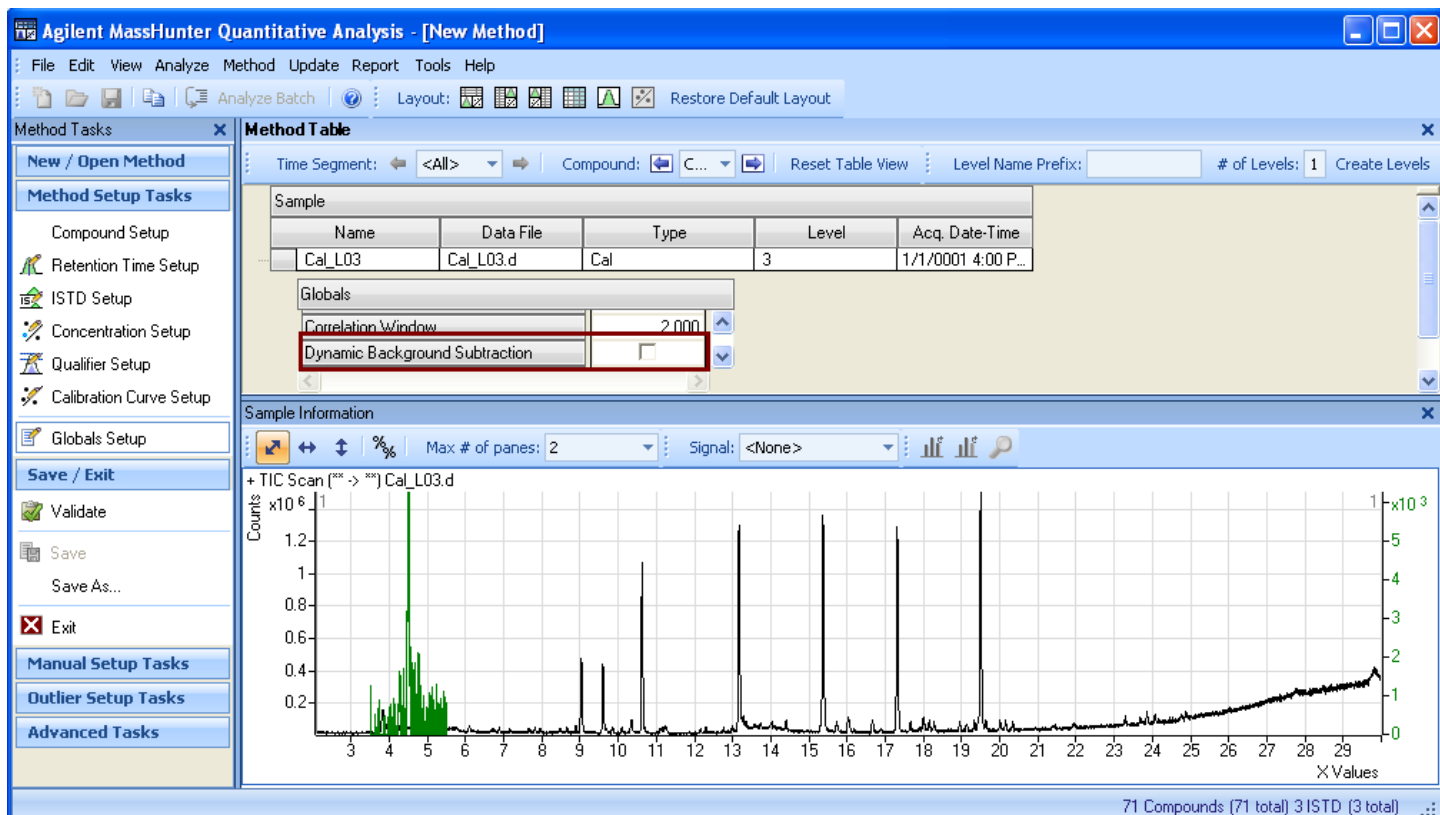
If the user opens a method from an existing batch, the DAMethodPathFileNameOrigin remains with its original setting. Note that if a user creates a method manually, the DAMethodPathFileNameOrigin is not set.

## DataVersion

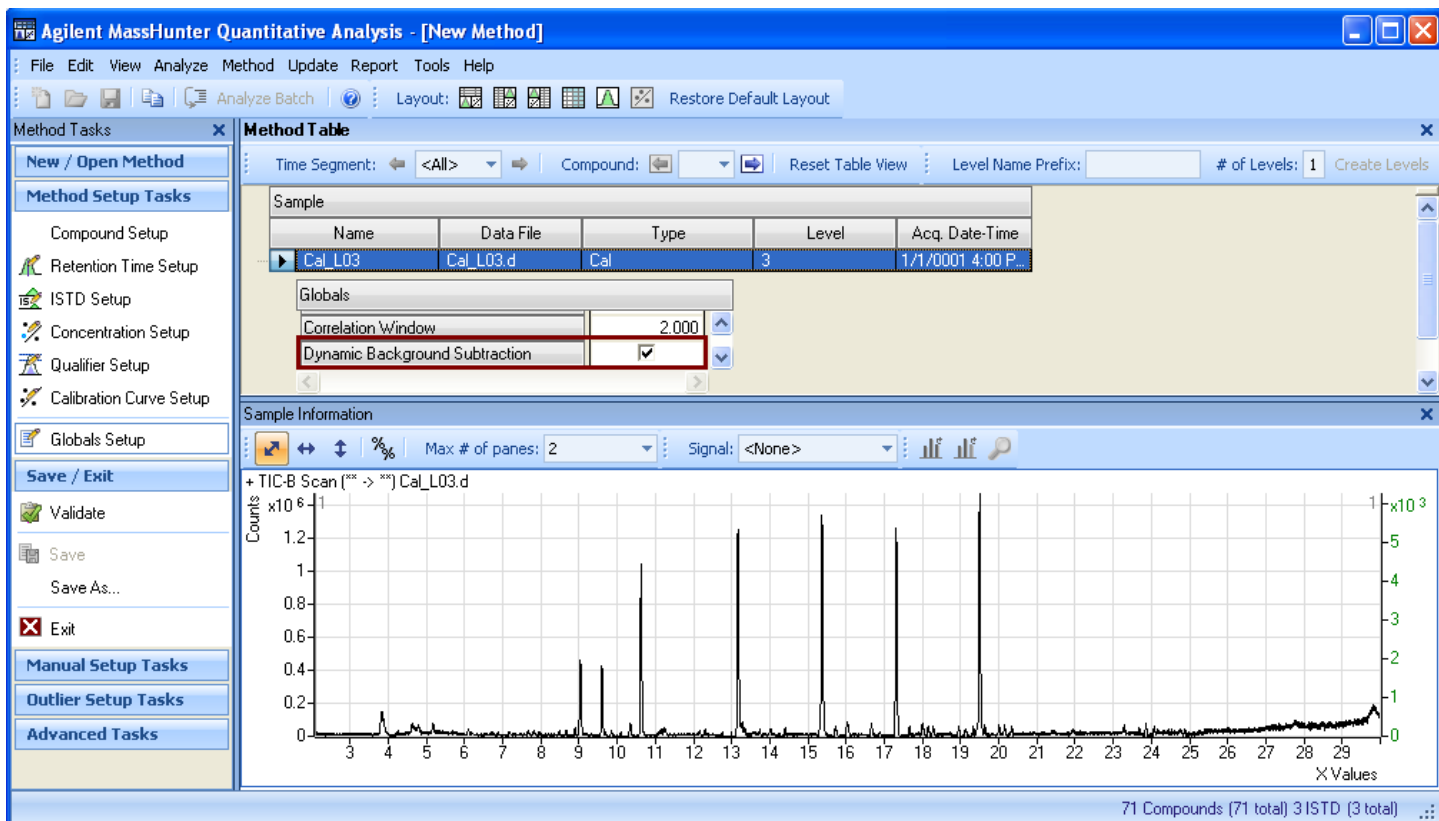
[DataVersion](#) represents the version of the software used to generate the reporting results.

## DynamicBackgroundSubtraction

[DynamicBackgroundSubtraction](#) “flattens” the chromatogram. DynamicBackgroundSubtraction activates an algorithm which processes the raw chromatogram by removing “noise” ions. “Noise” ions, which are evaluated by deconvolution technique, do not group together forming a peak shape and are therefore considered part of the background.



DBS 1: Quant Method globals allows DynamicBackgroundSubtraction which affects all chromatograms in batch.



DBS 2: Enabled DynamicBackgroundSubtraction "flattens" the chromatogram. Compare before and after.

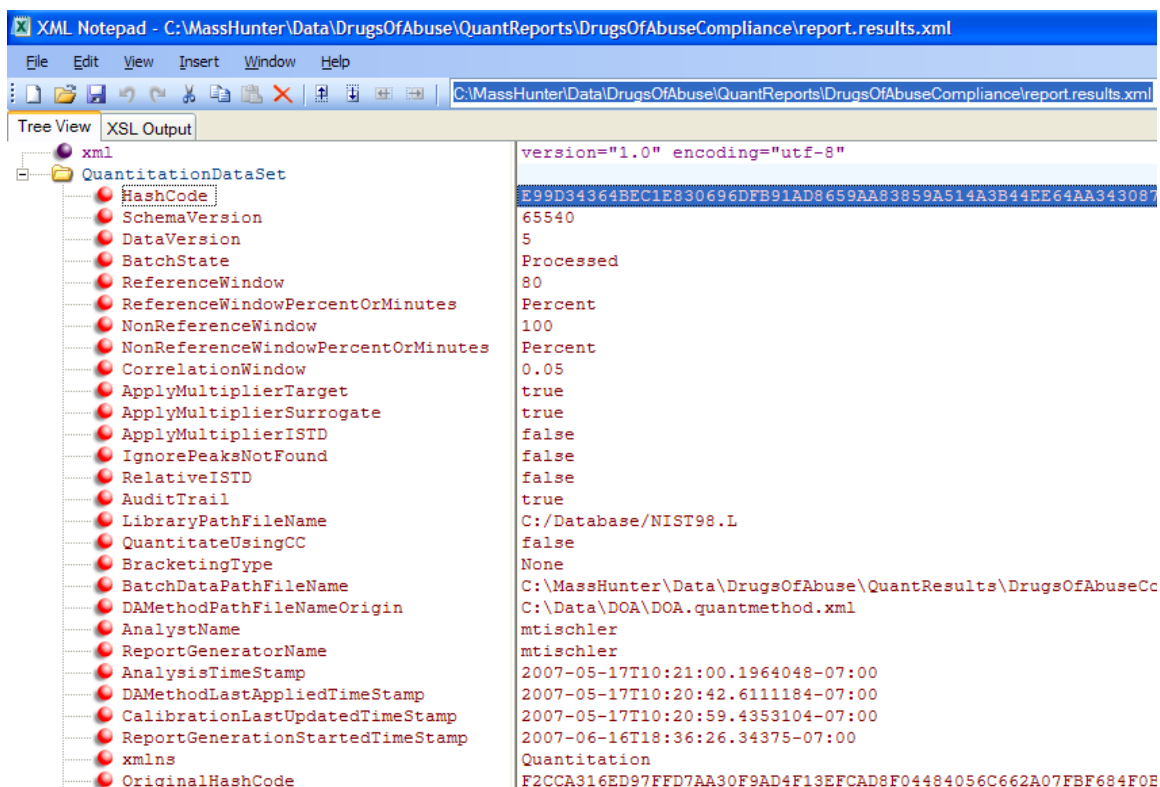
Note that DynamicBackgroundSubtraction requires computer time to execute the algorithm so enabling DynamicBackgroundSubtraction will slow down the Quant Analysis time.

# FeatureDetection

[FeatureDetection](#) changes the data access being used in quantitation. If it is true, feature data access (marketing name "SureMass") is used. It only applies to accurate mass data.

# HashCode

[HashCode](#) is a checksum calculated and stored with the results.



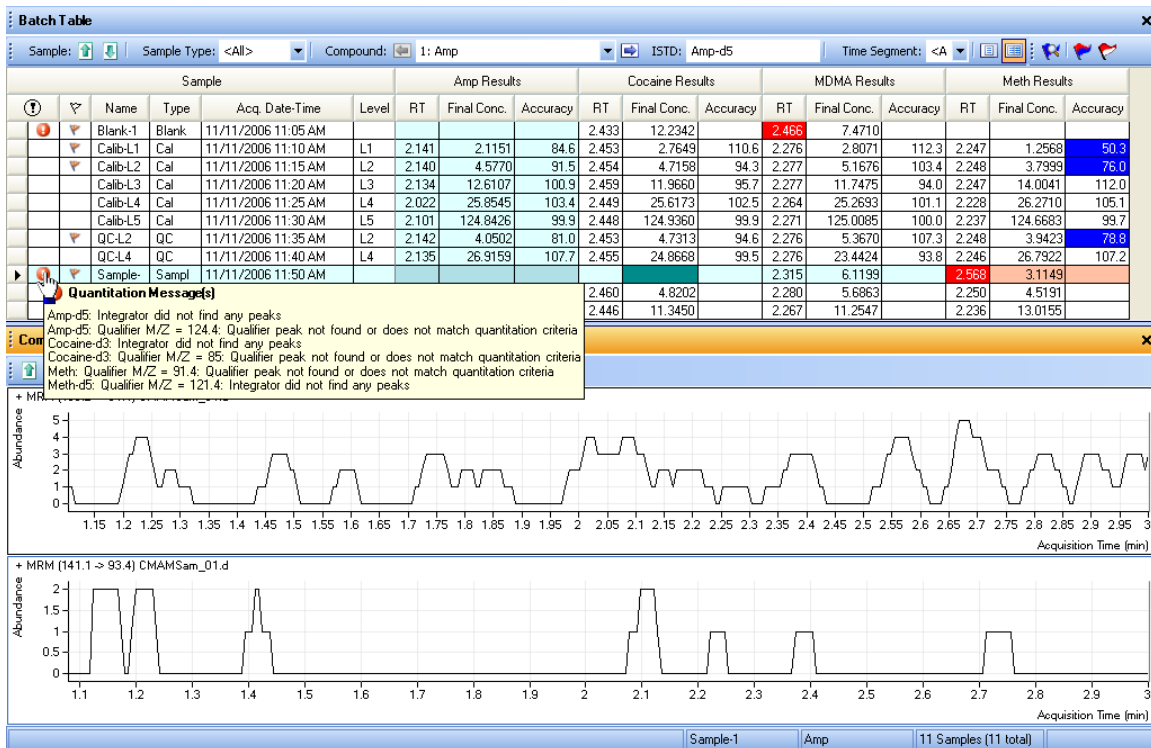
**Hashcode 1: Unique string stored in XML document identifies any changes to the document if the hash code does not match.**

# IgnorePeaksNotFound

[IgnorePeaksNotFound](#) is a global flag that affects the Quantitation Message. The purpose is avoid flagging target compounds that are normally absent in target samples, such as pesticides in food samples.

If the IgnorePeaksNotFound global flag is false, the software will flag all errors of type "Peak not found" with a Quantitation Message. If IgnorePeaksNotFound is true (the box is checked), the "Peak not found" quantitation message errors are ignored for target compounds in target samples (Sample) and blank samples (Blank, DoubleBlank, and MatrixBlank). Failed manual integrations, ISTD compounds, MatrixSpike compounds, Surrogate compounds and non-target samples are still flagged. ISTD compound in DoubleBlank sample is not flagged since it is not expected to be present.





**IgnorePeaksNotFound:** With this sample, analysis informs you with a quantitation message that for this particular compound, no peak has been found. If you do not want to see messages informing you that no peaks are found, you can turn on this batch global setting.

## LibraryMethodPathFileName

[LibraryMethodPathFileName](#) is the file system path and file name to the library method that contains parameter settings for deconvolution, library search and compound identification.

## LibraryPathFileName

[LibraryPathFileName](#) is the file system path and file name to the Agilent formatted compound library used during Library Search features. Library search features are disabled if the [LibrarySearchPathFileName](#) is NULL. This field is obsolete now.

# NonReferenceWindow

[NonReferenceWindow](#) is used to determine if the peak specified in the Quantitation DataSet is present in the data file currently being processed.

## Example:

A window of 5% means that the peak group (quantifier and qualifier peaks) processed must have an average retention time within +/-2.5% of the time in the quantitation database.

The reference window applies to internal standards that are designated as time reference peaks. The non-reference window applies to all other compounds.

The NonReferenceWindow size is based on the [NonReferenceWindowPercentOrMinutes](#).

## Example:

Changing the non-reference RT window from 40 percent to 200 percent increases the range around the expected RT that is used to identify quantifier peaks. The wider window helps with retention times that wander around from sample to sample.

Recognition window is the RT range around the adjusted expected Retention Time  $RT'$ . The RT range is determined from the ReferenceWindow size or NonReferenceWindow size depending on if the compound has a time reference compound or not. Adjusted expected Retention Time is equal expected Retention Time if the compound does not have a time reference ISTD; and is adjusted by the ratio of the actual-to-expected retention time of reference ISTD's primary hit peak if it has a time reference ISTD. i.e.,

*Recognition window = [  $RT' - 0.5 * ReferenceWindow Size$ ,  $RT' + 0.5 * ReferenceWindow Size$  ] or*

*Recognition window = [  $RT' - 0.5 * NonReferenceWindow Size$ ,  $RT' + 0.5 * NonReferenceWindow Size$  ]*

Note: If the ReferenceWindow size is smaller than the Correlation Window it is possible to see a target or qualifier peak that falls outside the ReferenceWindow. Recognition window is ignored when manual integration is performed.

## NonReferenceWindowPercentOrMinutes

[NonReferenceWindowPercentOrMinutes](#) represents the setting in percent or minutes for the non-reference window.

Enum Name	UI Name	XPath expression
Minutes	Minutes	*//@NonReferenceWindowPercentOrMinutes[.='Minutes']
Percent	Percent	*//@NonReferenceWindowPercentOrMinutes[.='Percent']

## ReferenceWindow

[ReferenceWindow](#) is used to determine if the peak specified in the Quantitation DataSet is present in the data file currently being processed.

### Example:

A window of 5% means that the peak group (quantifier and qualifier peaks) being processed must have an average retention time within +/-2.5% of the time in the quantitation database.

The reference window is used for internal standards that are designated as time reference peaks. The non-reference window is used for all other compounds.

The ReferenceWindow size is based on the [ReferenceWindowPercentOrMinutes](#).

Recognition window is the RT range around the adjusted expected Retention Time  $RT'$ . The RT range is determined from the ReferenceWindow size or NonReferenceWindow size depending on if the compound has a time reference compound or not. Adjusted expected Retention Time is equal expected Retention Time if the compound does not have a time reference ISTD; and is adjusted by the ratio of the actual-to-expected retention time of reference ISTD's primary hit peak if it has a time reference ISTD. i.e.,

*Recognition window = [  $RT' - 0.5 * ReferenceWindow Size$ ,  $RT' + 0.5 * ReferenceWindow Size$  ] or*

*Recognition window = [  $RT' - 0.5 * NonReferenceWindow Size$ ,  $RT' + 0.5 * NonReferenceWindow Size$  ]*

Note: If the ReferenceWindow size is smaller than the Correlation Window it is possible to see a target or qualifier peak that falls outside the ReferenceWindow. Recognition window is ignored when manual integration is performed.

## ReferenceWindowPercentOrMinutes

[ReferenceWindowPercentOrMinutes](#) represents the setting in percent or minutes for the reference window.

Enum Name	UI Name	XPath expression
Minutes	Minutes	*//@ReferenceWindowPercentOrMinutes[.='Minutes']
Percent	Percent	*//@ReferenceWindowPercentOrMinutes[.='Percent']

## RefLibraryPathFileName

[RefLibraryPathFileName](#) is the file system path and file name to the Reference Library created from high level calibration sample or from existing library in the .L or .mslibray.xml format. Reference Library Match score features are disabled if the RefLibrarySearchPathFileName is NULL.

## RefLibraryPatternPathFileName

[RefLibraryPatternPathFileName](#) is the file system path and file name to the Pattern Reference Library. The Pattern Reference Library is typically synthesized from the MolecularFormula and associated adducts and stores a "spectral" entry for each pattern.

More than one pattern is likely for each compound. For example, with the monoisotopic mass M, the isotopic patterns that corresponds to the (M+H)+ and (M+Na)+ and (M+K)+ adducts.

Note: Mass Match score features are disabled if the RefLibraryPatternPathFileName is NULL.

## RelativeISTD

[RelativeISTD](#) represents a mechanism to analyze using the ISTD as the reference calibration amount - instead of the typically ISTD correction.

In the following example, the amount of [Phe] is determined by calculating the area ratio against the heavy isotoped analog and then multiplying by the known ISTD amount of [D<sub>5</sub>Phe].

$$[Phe] = \frac{\text{Intensity of Phe}}{\text{Intensity of } D_5Phe} \times [D_5Phe]$$

Note that the RelativeISTD mechanism can adjust the Response Factor of the target versus ISTD using the [RelativeISTDMultiplier](#).

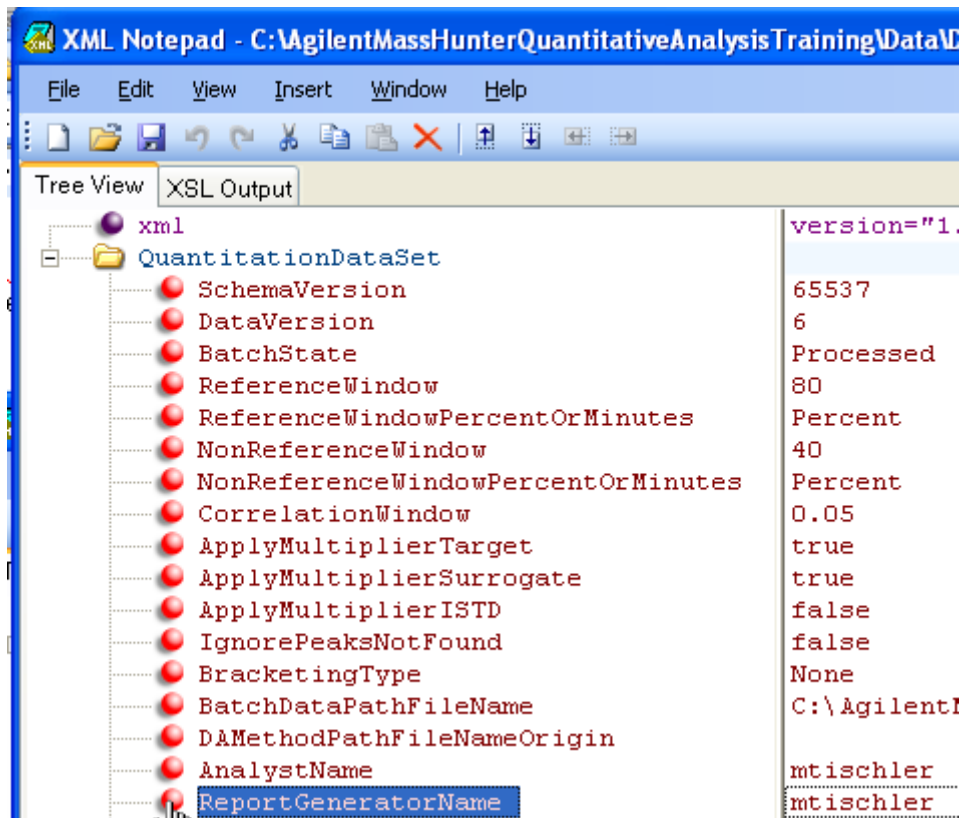
If Relative ISTD is checked in the Global Setup, then any individual ISTD concentrations that may have been entered in the calibration table are ignored and only the default ISTD concentration is used.

## ReportGenerationStartedTimeStamp

[ReportGeneratedStartedTimeStamp](#) is the date and time for initiation of reporting results generation. Value is updated in report.results.xml, instead of global.

# ReportGeneratorName

[ReportGeneratorName](#) records the user name that generated the reporting results.



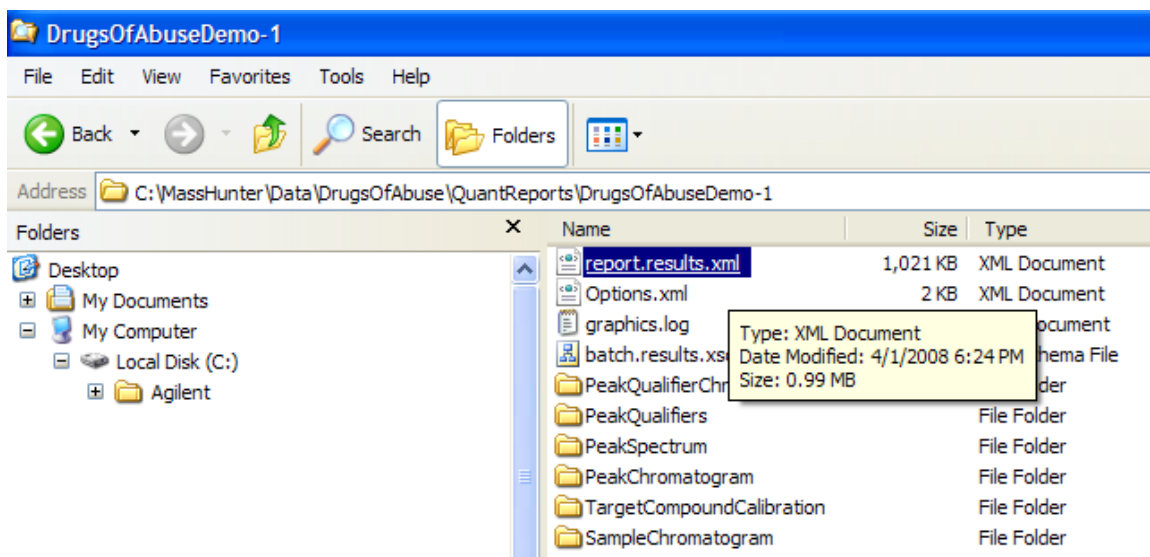
Name 2: Records user name.

# ReportQuantVersion

[ReportQuantVersion](#) designates the version of Quantitation software when report is generated.

# ReportResultsPathFileName

[ReportResultsPathFileName](#) is the file system path and file name to the reporting results generated. Uploading the reporting results sets the ReportResultsPathFileName so the location of the reporting results is known.



# RepositoryRevisionNumber

[RepositoryRevisionNumber](#) is the ECM batch revision number for Quant batch report.

# SchemaVersion

[SchemaVersion](#) designates the revision of the XML schema used with this particular Quantitation DataSet. The SchemaVersion is read from the batch XML file as an attribute and is compared to AppSchemaVersion.

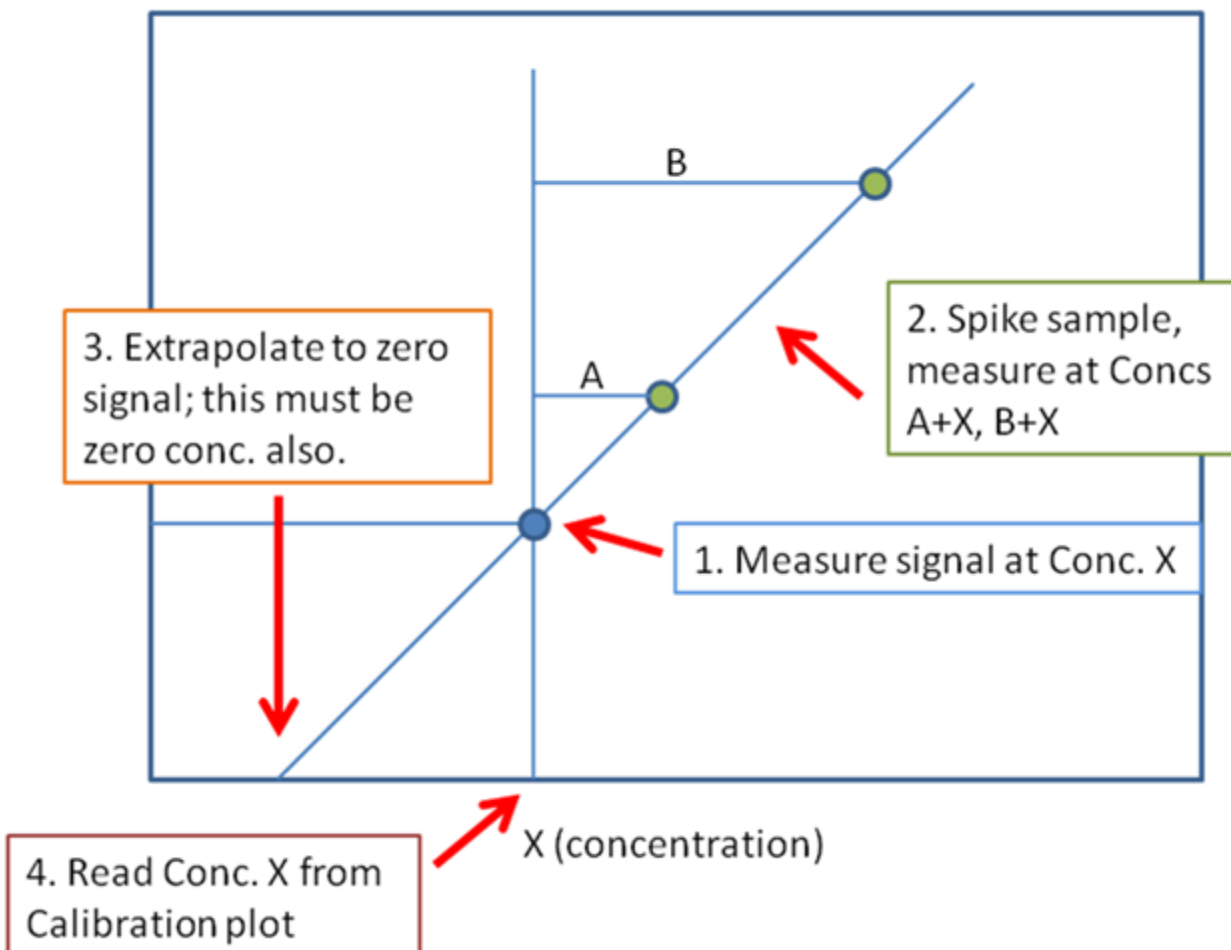
# Standard Addition

[Standard Addition](#) changes the association between samples and their "calibration" samples. The purpose of standard addition is to quantitate whenever the matrix of a sample changes the analytical sensitivity of the method.

Standard Addition is a technique that introduces a standard of your target compound directly into the analytical sample. After estimating the amount of target analyte present in the sample, samples are then spiked with known concentrations. By extrapolating the curve from the spiked samples, the original amount present in the sample can be determined. This technique assumes that the response for that particular analyte is linear in the concentration range of the sample.

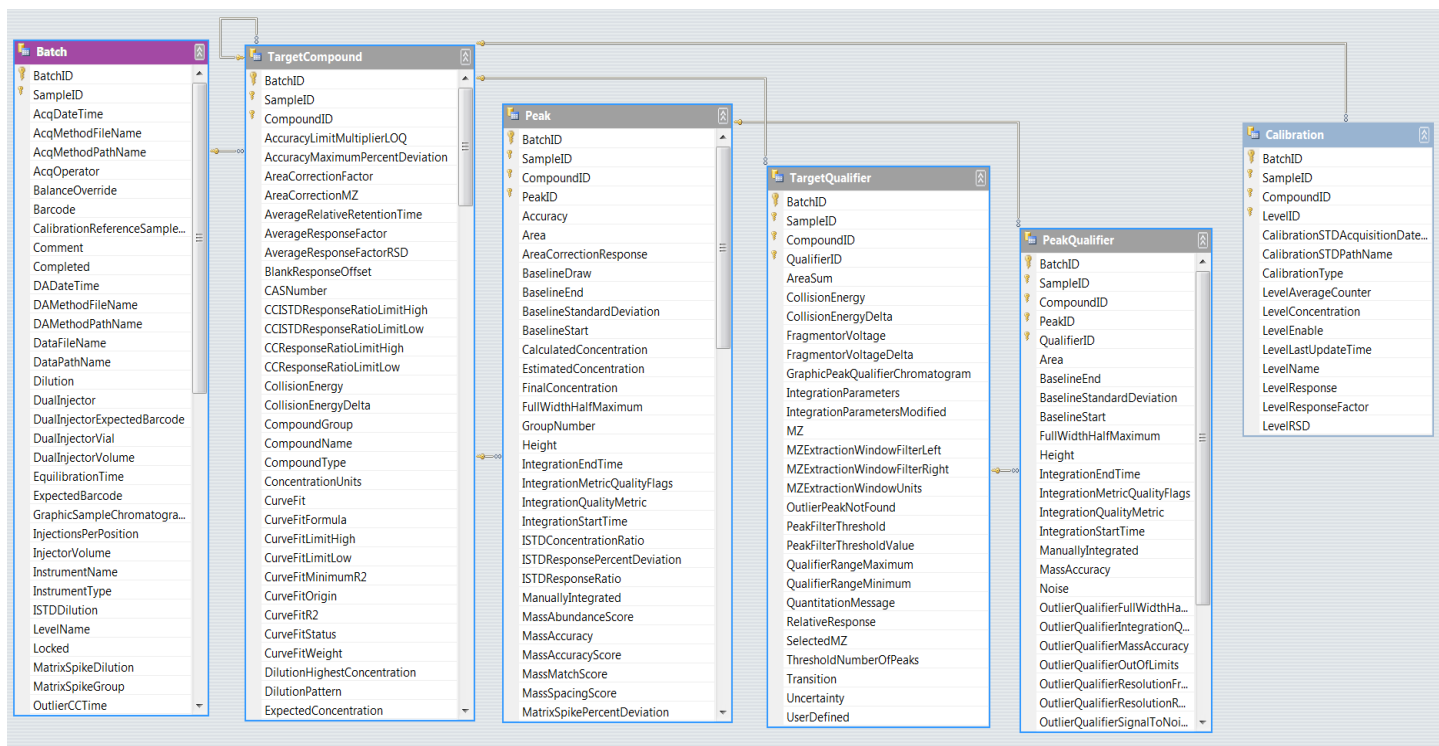
The purpose of the spiked standards is to establish an analytical curve and determine the response factor for the target analyte. With the responses obtained from the target analyte in both the original sample and the spiked samples,, the responses are used to calculate the method specific response factor for the target analyte. That response factor is subsequently used to determine the concentration of the unknown based on the responses of the unknown and the "standards".

## Standard Addition





# Batch Table



## Primary Key

{[BatchID](#), [SampleID](#)} serves as the primary key. The composite of the [BatchID](#) and [SampleID](#) uniquely identify each row in this table. The keys in the Quantitation DataSet are not shown in the user interface.

A primary key value must be unique within the table. A composite key is a primary key that incorporates more than one column.

## BatchID

[BatchID](#) uniquely identifies the batch. [BatchID](#) is part of the composite primary key. The [BatchID](#) is typically set to -1 because Batch-at-a-Glance analyzes one batch.

## SampleID

[SampleID](#) uniquely identifies the sample in the batch. [SampleID](#) is part of the composite primary key. Thus, each sample in the batch is assigned a unique [SampleID](#).

## AcqDateTime

[AcqDateTime](#) stores the date and time that the sample's raw data was acquired. It shows the date time where the Quant program is running.



A screenshot of a calendar for December 2006. The calendar is displayed in a grid format with days of the week (Sun, Mon, Tue, Wed, Thu, Fri, Sat) as columns and dates as rows. The date 4th is highlighted in blue. The calendar shows the following dates: 26, 27, 28, 29, 30, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 1, 2, 3, 4, 5, 6.

December, 2006						
Sun	Mon	Tue	Wed	Thu	Fri	Sat
26	27	28	29	30	1	2
3	4	5	6	7	8	9
10	11	12	13	14	15	16
17	18	19	20	21	22	23
24	25	26	27	28	29	30
31	1	2	3	4	5	6

## AcqDateTimeLocal

[AcqDateTimeLocal](#) records the acquisition date time in time zone where data is acquired.

## AcqMethodFileName

[AcqMethodFileName](#) stores the short filename of the acquisition method used to acquire the sample's raw data.

## AcqMethodPathName

[AcqMethodPathName](#) stores the path to the AcqMethodFileName used during acquisition.

## AcqOperator

[AcqOperator](#) stores the user that ran this sample.

## BalanceOverride

[BalanceOverride](#) stores sample information concerning the balance adjustments used during acquisition.

## Barcode

[Barcode](#) stores the sample information related to a Barcode identifier used during acquisition.

Barcode is a machine-readable representation of a string. Barcodes are typically used to labeled samples containers and scanned by optical scanners to "type" in the SampleName.



## CalibrationReferenceSampleID

[CalibrationReferenceSampleID](#) internally identifies the SampleID that contains the calibration table information.

The screenshot shows the 'Agilent MassHunter Quantitative Analysis - [New Method]' interface. The 'Method Table' pane displays the following data:

Quantifier				
Name	TS	Scan	Type	Units
Cocaine	1	MRM	Target	ng/ml

Calibration	
Level	Conc.
L1	2.5000
L2	5.0000
L2	5.0000
L3	12.5000
L4	25.0000
L4	25.0000
L5	125.0000

Figure 1: Show calibration table stored in QuantitationDataSet for a particular compound.

Note that the calibration table is stored in only one sample in the batch.

The only exceptions are cases where the calibration table is different for different sample such as [StandardAddition](#) or [BracketingType](#).

## Comment

[Comment](#) stores user entered information about this sample.

## Completed

[Completed](#) stores whether the sample was successfully finished acquisition.

## DADateTime

[DADateTime](#) stores the date and time that the sample's data was last processed.



A calendar widget for December 2006. The header shows "< December, 2006 >". The days of the week are listed as Sun, Mon, Tue, Wed, Thu, Fri, Sat. The dates are arranged in a grid. The date 4 is highlighted in blue.

Sun	Mon	Tue	Wed	Thu	Fri	Sat
26	27	28	29	30	1	2
3	4	5	6	7	8	9
10	11	12	13	14	15	16
17	18	19	20	21	22	23
24	25	26	27	28	29	30
31	1	2	3	4	5	6

## DAMethodFileName

[DAMethodFileName](#) stores the data analysis method name used to analyze this sample. If the method was not saved using a name, then DAMethodFileName is `NULL`.

## DAMethodPathName

[DAMethodPathName](#) stores the path to the Data Analysis Method name. If the method was not saved using a name, then DAMethodPathName is `NULL`.

Address		C:\Data\THC_in_Oral_Fluids\OF_THC_01.d\AcqData			
Folders	Name	Size	Type	Date Modified	
THC_in_Oral_Fluids	MSTS.xml	1 KB	XML Document	11/9/2005 7:24 PM	
OF_THC_01.d	AcqData	1 KB	File	11/9/2005 7:24 PM	
AcqData	MSScan.bin	249 KB	BIN File	11/8/2005 4:43 AM	
OF_THC_02.d	MSPeak.bin	27 KB	BIN File	11/8/2005 4:43 AM	
OF_THC_03.d	Worklist.xml	41 KB	XML Document	9/16/2005 4:29 AM	
OF_THC_04.d	MSScan.xsd	4 KB	XML Schema File	5/26/2005 1:36 PM	

DAMethodPathName: This DAMethodPathName is C:\Data\THC\_in\_Oral\_Fluids\.

## DataFileName

[DataFileName](#) stores the name of the data file directory (.d) that collects this sample's files.

Address		C:\Data\THC_in_Oral_Fluids\OF_THC_01.d\AcqData			
Folders	Name	Size	Type	Date Modified	
THC_in_Oral_Fluids	MSTS.xml	1 KB	XML Document	11/9/2005 7:24 PM	
OF_THC_01.d	AcqData	1 KB	File	11/9/2005 7:24 PM	
AcqData	MSScan.bin	249 KB	BIN File	11/8/2005 4:43 AM	
OF_THC_02.d	MSPeak.bin	27 KB	BIN File	11/8/2005 4:43 AM	
OF_THC_03.d	Worklist.xml	41 KB	XML Document	9/16/2005 4:29 AM	
OF_THC_04.d	MSScan.xsd	4 KB	XML Schema File	5/26/2005 1:36 PM	

DataFileName: The DataFileName for this sample is OF\_THC\_01.d.

## DataPathName

[DataPathName](#) stores the path to the DataFileName. It's the location of data when samples were originally added to the batch.

Address		C:\Data\THC_in_Oral_Fluids\OF_THC_01.d\AcqData			
Folders	Name	Size	Type	Date Modified	
THC_in_Oral_Fluids	MSTS.xml	1 KB	XML Document	11/9/2005 7:24 PM	
OF_THC_01.d	AcqData	1 KB	File	11/9/2005 7:24 PM	
AcqData	MSScan.bin	249 KB	BIN File	11/8/2005 4:43 AM	
OF_THC_02.d	MSPeak.bin	27 KB	BIN File	11/8/2005 4:43 AM	
OF_THC_03.d	Worklist.xml	41 KB	XML Document	9/16/2005 4:29 AM	
OF_THC_04.d	MSScan.xsd	4 KB	XML Schema File	5/26/2005 1:36 PM	

DataPathName: This DataPathName is C:\Data\THC\_in\_Oral\_Fluids\.

## Dilution

[Dilution](#) stores the Dilution Factor.

*Multiplier = Dilution*

*FinalConcentration = CalculatedConcentration × Multiplier*

### **Example:**

If the sample is diluted by a factor of 2, the Dilution Factor is 2. Hence, the [CalculatedConcentration](#) is multiplied by 2 to adjust the [FinalConcentration](#).

## DualInjector

[DualInjector](#) declares that another vial is injected in the other injector port during the sample run. The dual injection expects an acquired signal used for confirmation. The dual signal is stored in the same .d as the sample acquired.

Since one sample is organized as one .d directory, analysis typically treats the signal as acquired from the same sample.

## DualInjectorAcqDateTime

[DualInjectorAcqDateTime](#) stores the date and time that the sample's raw data was acquired from the dual injector. It shows the date time where the Quant program is running.

## DualInjectorBarcode

[DualInjectorBarcode](#) stores the sample information related to the Barcode identifier used during acquisition for the dual injector.

Barcode is a machine-readable representation of a string. Barcodes are typically used to labeled samples containers and scanned by optical scanners to "type" in the SampleName.



## DualInjectorExpectedBarcode

[DualInjectorExpectedBarcode](#) stores the sample information related to a Barcode identifier used during acquisition. The DualInjector typically refers to the rear GC injector as opposed to the front GC injector i.e. [ExpectedBarcode](#).

## DualInjectorVial

[DualInjectorVial](#) stores the number of the vial used to create the dual injection.

## DualInjectorVolume

[DualInjectorVolume](#) stores the volume of the dual injection for this sample.

## EquilibrationTime

[EquilibrationTime](#) stores the time used to equilibrate the column before injection.

## ExpectedBarcode

[ExpectedBarcode](#) stores the sample information related to a Barcode identifier used during acquisition.

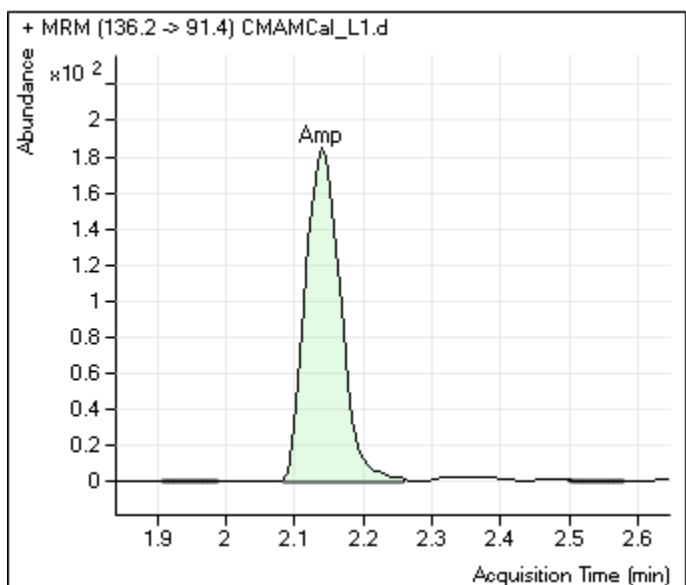
[ExpectedBarcode](#) stores the barcode recorded during sample login which typically matches the [BarCode](#).

ExpectedBarcode is a machine-readable representation of a string. Barcodes are typically used to label samples containers and are scanned by optical scanners to "type" in the SampleName.



## GraphicSampleChromatogram

[GraphicSampleChromatogram](#) represents a relative path and filename to a graphic (.emf) file used in reporting.



**Graphic 1: Graphic file reference.**



## InjectionsPerPosition

[InjectionsPerPosition](#) stores the number of injections from that particular position in that container. A typical container is a vial.

Not necessarily support in all acquisition subsystems.

## InjectorVolume

[InjectorVolume](#) stores the volume of the injection for this sample.

## InstrumentName

[InstrumentName](#) stores the name of the instrument that acquired this sample.

InstrumentName is useful to relate back to the instrument used to answer questions about the acquired data origins.

## InstrumentType

[InstrumentType](#) stores kind of instrument. Typical instruments are QQQ, qTOF, and TOF.

Different InstrumentTypes required different presentations. For example, MS/MS instruments have additional scan types.

# ISTDDilution

[ISTDDilution](#) stores a per sample [ISTDConcentration](#) correction.

*ISTDConcentration = ISTDDilution \* ISTDConcentration* (ISTD compound)

ISTDDilution is useful when you are weighing out the ISTD for each sample and the amount varies slightly.

ISTDDilution is also useful to correct for (mistakenly) adding twice as much ISTD as needed.

ISTDDilution updates the [ISTDConcentration](#) stored with the target compound that uses that ISTD compound.

ISTDDilution works independently from the [Multiplier](#) or [ApplyMultipliertoISTD](#) adjustments.

# MatrixSpikeDilution

[MatrixSpikeDilution](#) stores a per sample [MatrixSpike Concentration](#) correction. It only affects MatrixSpike expected concentration and MatrixSpike recovery. The CalculatedConcentration and FinalConcentration of MatrixSpike compound are not affected.

*MatrixSpike Concentration = MatrixSpike Dilution \* MatrixSpike Concentration (MatrixSpike Compound)*

MatrixSpikeDilution is useful when you are weighing out the MatrixSpike for each sample and the amount varies slightly.

MatrixSpikeDilution updates the [MatrixSpike Concentration](#) stored with the matrix spike compound.

# MatrixSpikeGroup

[MatrixSpikeGroup](#) represents a user-defined name that enables a set of samples to associate together in order to accomplish the [Matrix Spike Percent Recovery](#) calculations.

If MatrixSpikeGroup is assigned for any sample only this recovery outline is calculated.

# MatrixType

[MatrixType](#) is a user-defined name that enables association with MatrixTypeOverride to define different outlier limits at a per sample base.

# LevelName

[LevelName](#) stores the calibration level name used to identify the compound's concentrations into a group. LevelName(s) are used to identify Calibration and QC (Quality Control) samples that are used to construct the calibration curve for each compound. Different compounds can have different calibration levels with one restriction: Any internal standards must have the same number of levels, level names, and concentrations as the target compound.

The LevelName and the compound's [ExpectedConcentration](#) work together to establish the calibration curve.

LevelName(s) are established either during:

- Acquisition Sequence (Worklist) Setup

- Analysis time

LevelName is editable in Batch-at-a-Glance.

## Locked

[Locked](#) stores the "Locked" state of the Worklist during acquisition. If Locked is true then this sample was acquired under "Locked" acquisition Worklist conditions.

## PlateCode

[PlateCode](#) stores the code that identifies that plate (container).






PlateCode is sample information entered in acquisition.

## PlatePosition

[PlatePosition](#) stores the position that identifies to location on the plate (container).

## QuantitationMessage

[QuantitationMessage](#) stores problems associate with the analysis of that particular sample.

		CMAMStd_20.d	Sample		136.2 -> 91.4
		<b>Quantitation Message(s)</b>			91.4
	Cocaine-d0: Qualifier M/Z = 82: Integrator did not find any peaks				

## RackCode

[RackCode](#) stores the code that identifies the rack (container).

RackCode is sample information entered in acquisition.

## RackPosition

[RackPosition](#) stores the position in the rack (container).

RackCode is sample information entered in acquisition.

## RunStartValvePositionDescription

[RunStartValvePositionDescription](#) stores the LC column switching valve position at the start of the chromatographic run. Valve position determines which LC column is being used for chromatographic separation. Refer to the instrument LC column configuration for more information on this parameter.



## RunStartValvePositionNumber

[RunStartValvePositionNumber](#) stores the LC column switching valve position description at the start of the chromatographic run. Valve position determines which LC column is being used for chromatographic separation. Refer to the instrument LC column configuration for more information on this parameter.

## RunStopValvePositionDescription

[RunStopValvePositionDescription](#) stores the LC column switching valve position at the end of the chromatographic run. Valve position determines which LC column is being used for chromatographic separation. Refer to the instrument LC column configuration for more information on this parameter.

# RunStopValvePositionNumber

[RunStopValvePositionNumber](#) stores the LC column switching valve position description at the end of the chromatographic run. Valve position determines which LC column is being used for chromatographic separation. Refer to the instrument LC column configuration for more information on this parameter.

# SampleAmount

[SampleAmount](#) stores the amount of sample actually used in analysis. The SampleAmount along with the [TotalSampleAmount](#) computes the Multiplier. The Multiplier then converts the [CalculatedConcentration](#) to the [FinalConcentration](#).

$$\text{Multiplier} = \text{TotalSampleAmount} \div \text{SampleAmount}$$

$$\text{FinalConcentration} = \text{CalculatedConcentration} \times \text{Multiplier}$$

In this scenario, [FinalConcentration](#) adjusts as an amount.

## Example:

If your sample preparation needs to adjust the [FinalConcentration](#) for a volume, use the SampleAmount as the Volume adjustment and set TotalSampleAmount to "1".

$$\text{Multiplier} = 1 \div \text{SampleAmount}$$

Note that both SampleAmount and [TotalSampleAmount](#) must have values for the calculation to occur.

## Example:

If you need to adjust the [FinalConcentration](#) using several sample preparation factors, note that [Dilution](#) can work in concert with the TotalSampleAmount/SampleAmount adjustment.

$$\text{Multiplier} = (\text{TotalSampleAmount} \div \text{SampleAmount}) * \text{Dilution}$$

# SampleApproved

[SampleApproved](#) records the user's decision on the status of the sample. For example, the user sets the SampleApproved status to True, meaning the sample is considered approved.

SampleApproved is initialized to NULL and editable by the user in Batch-at-a-Glance.

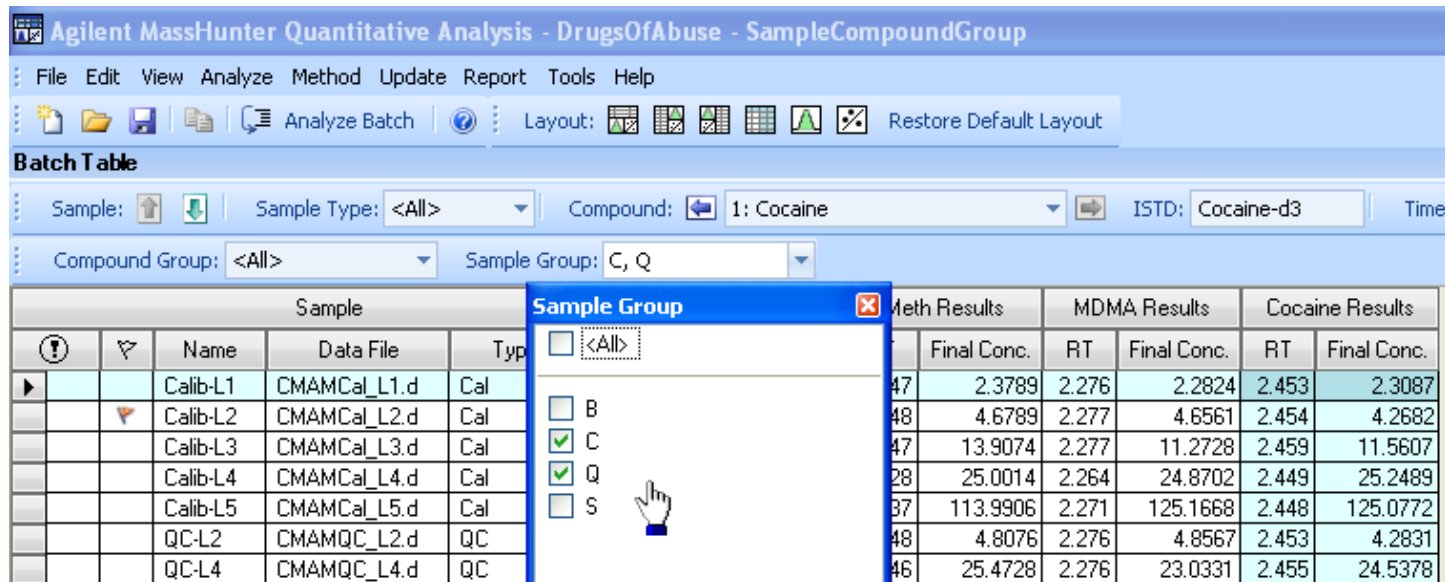
# SampleGroup

[SampleGroup](#) represents a user-defined name that enables a set of samples to associate together.

For example, if you create a sequence with a set of samples designated with the same SampleGroup name, then you could group those samples in reporting.

Another example, if you queued several different sequences together, yet with different SampleGroup names, then you could later search for those sequences using the SampleGroup column.

The quantitation software does not assign any particular behavior to the SampleGroup column so its purpose is user-defined.



The screenshot shows the Agilent MassHunter Quantitative Analysis interface. The title bar reads "Agilent MassHunter Quantitative Analysis - DrugsOfAbuse - SampleCompoundGroup". The menu bar includes File, Edit, View, Analyze, Method, Update, Report, Tools, and Help. The toolbar contains icons for file operations and a "Layout:" dropdown. The "Batch Table" section has controls for Sample, Sample Type, Compound (set to "1: Cocaine"), ISTD (set to "Cocaine-d3"), Compound Group, and Sample Group (set to "C, Q").

Sample					Sample Group	Meth Results		MDMA Results		Cocaine Results	
?	▼	Name	Data File	Type	<All>	Final Conc.	RT	Final Conc.	RT	Final Conc.	
▶		Calib-L1	CMAMCal_L1.d	Cal	<input type="checkbox"/> <All>	47	2.3789	2.276	2.2824	2.453	2.3087
	▼	Calib-L2	CMAMCal_L2.d	Cal	<input type="checkbox"/> B	48	4.6789	2.277	4.6561	2.454	4.2682
		Calib-L3	CMAMCal_L3.d	Cal	<input checked="" type="checkbox"/> C	47	13.9074	2.277	11.2728	2.459	11.5607
		Calib-L4	CMAMCal_L4.d	Cal	<input checked="" type="checkbox"/> Q	28	25.0014	2.264	24.8702	2.449	25.2489
		Calib-L5	CMAMCal_L5.d	Cal	<input type="checkbox"/> S	37	113.9906	2.271	125.1668	2.448	125.0772
		QC-L2	CMAMQC_L2.d	QC		48	4.8076	2.276	4.8567	2.453	4.2831
		QC-L4	CMAMQC_L4.d	QC		46	25.4728	2.276	23.0331	2.455	24.5378

**SampleGroup 1:** Labeling samples with a SampleGroup name enables customizable filtering.

# SampleInformation

[SampleInformation](#) stores the information about the sample.

SampleInformation is sample information entered in acquisition.

## SampleName

[SampleName](#) stores the name of the sample.

SampleName is sample information entered in acquisition.

## SamplePosition

[SamplePosition](#) stores the position of the sample.

In LC-MS acquisition, the SamplePosition typically stores the position of the sample in the container.

SamplePosition is sample information entered in acquisition.

## SamplePrepFileName

[SamplePrepFileName](#) stores the filename of the sample preparation method used when running this particular sample.

## SamplePrepPathName

[SamplePrepFile](#) stores the path i.e. directory of the sample preparation method used when running this particular sample.

## SampleState

[SampleState](#) stores the state of the sample.

Typical definitions are as follows:

Entered— Sample entered in a sample tracking



Analyzed— Sample analyzed by Quantitative Analysis

# SampleType

[SampleType](#) stores the type of sample.

Typical definitions are as follows:

**Sample**—the actual matrix (i.e. water, soil, food, etc.) which possibly contains the compound(s) of interest in unknown quantities as prepared for analysis (i.e. sample preparation). For Drug mode workflow, this sample type is referred to as a “Specimen”.

**Blank**—usually an amount of the solvent(s) used for preparation of the sample that is analyzed in order to detect possible contamination. ISTD is added to this sample to allow proper quantitation. For Drug mode workflow, this sample type is referred to as a “Negative”.

**Double Blank**—identical to a blank above except the Internal Standard is not added to it. For Drug mode workflow, this sample type is referred to as a “Blank”.

**Calibration Sample (aka Standard)**—an amount of solvent(s) that contains a known quantity of the compound(s) of interest. Calibration Samples are injected at different levels to construct a Calibration Curve.

**QC Sample** — an amount of solvent(s) that contains a known quantity of the compound(s) of interest (just like a Calibration Sample). The QC Sample is injected and quantitated like a regular Sample in order to validate the Calibration Curve.

**CC Sample** — an amount of solvent(s) that contains a known quantity of the compound(s) of interest (just like a QC Sample). The CC Sample is injected and quantitated like a regular Sample in order to validate the initial Calibration Curve. If the initial Calibration Curve is acceptable, then the Calibration Curve is considered satisfactory and re-running the Calibration sample is not considered necessary.

**Matrix Blank**—an amount of the matrix (i.e. water, soil, food, etc.) which is known to not have any of the compound(s) of interest that is prepared for analysis (i.e. sample preparation).

**Matrix QC (aka Matrix Spike)** —an amount of the matrix (i.e. water, soil, food, etc.) which is “spiked” with a known amount of the compound(s) of interest and then prepared for analysis (i.e. sample preparation). A parameter called the “Recovery” is calculated from the Matrix QC to measure the accuracy of the analysis.

**Matrix QC Duplicate (aka Matrix Spike Duplicate)** —identical to a Matrix QC, the term is used when two Matrix QC of the same concentration are quantitated to validate the precision of the analysis (i.e. that you can inject the identical amount twice and get the same results).

**ISTD (“Internal Standard”)**—a compound with similar chemical characteristics but different physical characteristics (e.g. m/z) than the compound(s) of interest that is “spiked” into all the Sample Types. The ISTD is then used to correct concentrations for all Sample Types based on its concentration. It may also be used to adjust the retention times of the compound(s) of interest if its retention time shifts during a set of analyses.

**Surrogate**—identical to an ISTD except it is not used to correct concentrations for all Sample

Types based on its concentration.

SampleType is editable in Batch-at-a-Glance.

Enum Name		XPath expression
Sample		*//SampleType[.='Sample']
Blank		*//SampleType[.='Blank']
Calibration		*//SampleType[.='Calibration']
QC		*//SampleType[.='QC']
CC		*//SampleType[.='CC']
DoubleBlank		*//SampleType[.='DoubleBlank']
Matrix		*//SampleType[.='Matrix']
MatrixDup		*//SampleType[.='MatrixDup']
MatrixBlank		*//SampleType[.='MatrixBlank']
TuneCheck		*//SampleType[.='TuneCheck']
ResponseCheck		*//SampleType[.='ResponseCheck']

## SamplingDateTime

[SamplingDateTime](#) holds the date and time that enables a time relationship between samples in the batch.

Certain time series experiments involve sampling at time intervals to monitor changes in analytes. Recording the SamplingDateTime enables the organization of the samples in a time-oriented sequence.

For example, in biological systems, a time series study involves monitoring the metabolite concentration levels over time after administration of an antagonist.

## SamplingTime

[SamplingTime](#) stores time measured as a number in arbitrary units.

For example, seconds since the initiation of an experiment.  
Recording SamplingTime is useful in a time-series sampling.

## SequenceFileName

[SequenceFileName](#) stores the sequence file name that was used to acquire the sample's raw data.

## SequencePathName

[SequencePathName](#) stores the sequence path name that was used to acquire the sample's raw data.

## SurrogateDilution

[SurrogateDilution](#) stores a per sample [Surrogate Concentration](#) correction. It only affects Surrogate expected concentration and surrogate recovery. The CalculatedConcentration and FinalConcentration of surrogate compound are not affected.

$$\text{Surrogate Concentration} = \text{Surrogate Dilution} * \text{Surrogate Concentration} \text{ (Surrogate Compound)}$$

SurrogateDilution is useful when you are weighing out the surrogate for each sample and the amount varies slightly.

SurrogateDilution updates the [Surrogate Concentration](#) stored with the surrogate compound.

SurrogateDilution works independently from the [Multiplier](#) or ApplyMultipliertoS surrogate adjustments.

## TrayName

[TrayName](#) stores the tray name.

Typical the trayname refers to the CTC PAL injector tray.

## TotalSampleAmount

[TotalSampleAmount](#) stores the total amount of the sample. The [SampleAmount](#) in conjunction with the TotalSampleAmount adjusts the [FinalConcentration](#).

$$\text{Multiplier} = \text{TotalSampleAmount} \div \text{SampleAmount}$$

$$\text{FinalConcentration} = \text{CalculatedConcentration} \times \text{Multiplier}$$

In this scenario, [FinalConcentration](#) adjusts as an amount.

## TuneFileLastTimeStamp

[TuneFileLastTimeStamp](#) stores the last tune time of the instrument that was used to acquire the sample's raw data. It's the time stamp of the tune file whose file name is TuneFileName.

## TuneFileName

[TuneFileName](#) stores the tune filename that was used to tune the instrument when acquire the sample's raw data.

## TunePathName

[TunePathName](#) stores the path name of the tune file that was used to tune the instrument when acquire the sample's raw data.

## UserDefined

[UserDefined](#) stores an arbitrary user-defined string.

UserDefined is editable in Batch-at-a-Glance.

## UserDefined1

[UserDefined1](#) stores an arbitrary user-defined string.

## UserDefined2

[UserDefined2](#) stores an arbitrary user-defined string.

## UserDefined3

[UserDefined3](#) stores an arbitrary user-defined string.

## UserDefined4

[UserDefined4](#) stores an arbitrary user-defined string.

## UserDefined5

[UserDefined5](#) stores an arbitrary user-defined string.

## UserDefined6

[UserDefined6](#) stores an arbitrary user-defined string.

## UserDefined7

[UserDefined7](#) stores an arbitrary user-defined string.

## UserDefined8

[UserDefined8](#) stores an arbitrary user-defined string.

## UserDefined9

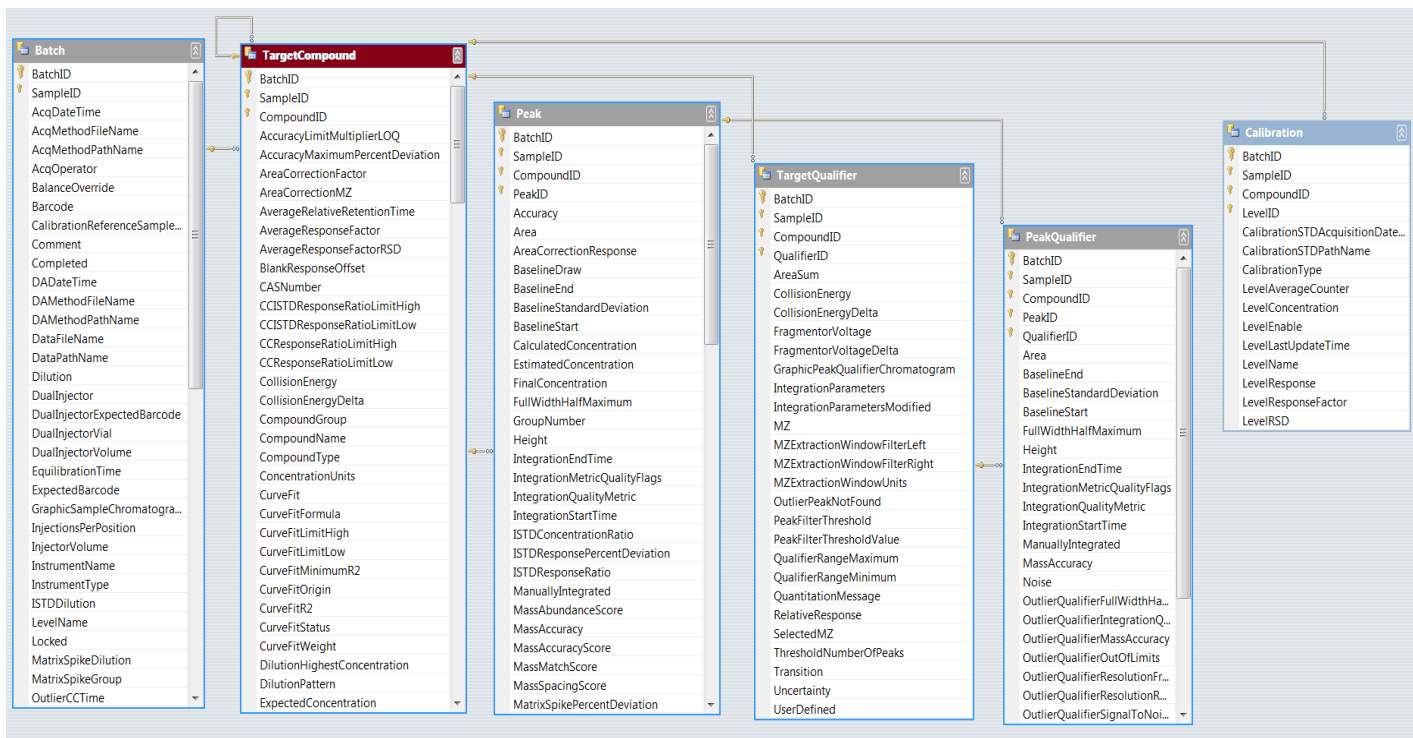
[UserDefined9](#) stores an arbitrary user-defined string.

## Vial

[Vial](#) stores the number or designator that identifies the vial used to create the injection.

In GC-MS acquisition, the Vial typically stores the sample vial number for the container.

# TargetCompound Table



## Primary Key

{[BatchID](#), [SampleID](#), [CompoundID](#)} serves as the primary key. The composite of the [BatchID](#) and [SampleID](#) and [CompoundID](#) unique identify each row in this table. The keys in the Quantitation DataSet are not show in the user interface.

A primary key value must be unique with in the table. A composite key is a primary key that incorporates more than one column.

## BatchID

[BatchID](#) uniquely identifies the batch. BatchID is part of the composite primary key. The BatchID is typically set to -1 because Batch-at-a-Glance analyzes one batch.

## SampleID

[SampleID](#) uniquely identifies the sample in the batch. SampleID is part of the composite primary key. Thus, each sample in the batch is assigned a unique SampleID.

## CompoundID



[CompoundID](#) uniquely identifies the sample in the batch. CompoundID is part of the composite primary key. Thus, each compound in the batch is assigned a unique CompoundID.

## AccuracyLimitMultiplierLOQ

[AccuracyLimitMultiplierLOQ](#) represents an adjustment to lowest enabled calibration level Accuracy limit.

### Example:

If AccuracyMaximumPercentDeviation is set at 20% and AccuracyLimitMultiplierLOQ is set at 1.5, the lowest enabled calibration level Accuracy is evaluated with the limit of 30%.

## AccuracyMaximumPercentDeviation

[AccuracyMaximumPercentDeviation](#) represents the limit for the Accuracy outlier. [OutlierAccuracy](#) is set to High if this compound's [CalculatedConcentration](#) exceeds ExpectedConcentration by more than AccuracyMaximumPercentDeviation percent.

## AgilentID

[AgilentID](#) represents an identifier in Agilent database.

## AlternativePeakCriteria

[AlternativePeakCriteria](#) represents a standard, e.g., deconvoluted library match score, to evaluate the quality of an alternative peak against the primary peak selected by Quant engine.

## AlternativePeakID

[AlternativePeakID](#) represents the peak ID of an alternative peak that has better score based on the [AlternativePeakCriteria](#) selected.

## AreaCorrectionFactor

[AreaCorrectionFactor](#) represents a scale factor. AreaCorrectionFactor is applied to the integrator-determined area of an Area Correction signal specified by AreaCorrectionMZ. The resulting product is subtracted from the integrator-determined area of the signal specified by MZ (and SelectedMZ in the case of tandem mass spectral experiments). The resulting difference is used for target signal response quantitation. If QuantitateByHeight is true, area correction is based on peak height.

## AreaCorrectionMZ

[AreaCorrectionMZ](#) represents a mass-to-charge measurement, in units of daltons per unit charge, which specifies a signal to extract from the quantitation data source. Once extracted, this signal is integrated and the resulting area is subtracted from the target signal area. The resulting difference is used for quantitation instead of the unmodified target signal area. If the value of [AreaCorrectionMZ](#) is 0, no area-correction signal is extracted, and no area correction is brought to bear on the target signal response. If [QuantitateByHeight](#) is true, area correction is based on peak height.

## AreaCorrectionSelectedMZ

[AreaCorrectionSelectedMZ](#) together with [AreaCorrectionMZ](#) defines a MRM signal to extract from the quantitation data source. Once extracted, this signal is integrated and the resulting area is subtracted from the target signal area. The resulting difference is used for quantitation instead of the unmodified target signal area. If the value of [AreaCorrectionMZ](#) is 0, no area-correction signal is extracted, and no area correction is brought to bear on the target signal response. If [QuantitateByHeight](#) is true, area correction is based on peak height.

## AverageRelativeRetentionTime

[AverageRelativeRetentionTime](#) represents the average of the relative retention time values of all the peaks that provide the responses for this compound's enabled Calibration and QC points. A relative retention time is defined as the ratio of the retention time of the primary peak for the target compound to the retention time of the primary peak of the related internal standard. [AverageRelativeRetentionTime](#) is computed only for those compounds that have an internal standard. [AverageRelativeRetentionTime](#) is used to evaluate the Relative Retention Time outlier condition.

## AverageResponseFactor

[AverageResponseFactor](#) represents the average of the response factors of all the enabled calibration points for this compound. The response factor of a calibration point is defined as the ratio of the calibration peak's response to the concentration of this point's calibration level. [AverageResponseFactor](#) is used to evaluate to the Average Response Factor outlier condition.

## AverageResponseFactorRSD

[AverageResponseFactorRSD](#) represents the relative standard deviation of the level response factors of a target compound across the calibration levels. AverageResponseFactor RSD is used to evaluate to the Average Response Factor RSD outlier condition.

## BlankResponseOffset

[BlankResponseOffset](#) stores the average of the TargetResponse values for the same compound in all the samples of type Blank. If there are no blank samples in the batch, the column stays NULL.

## CalibrationRangeFilter

[CalibrationRangeFilter](#) is an enum {HighOnly, LowOnly, HighLow} that controls what flag to show for Calibration range outlier.

## CalibrationReferenceCompoundID

[CalibrationReferenceCompoundID](#) is the CompoundID of the compound whose calibration curve is inherited by current compound.

## CapacityFactorLimit

[CapacityFactorLimit](#) is the outlier limit for the capacity factor outlier.

# CASNumber

[CASNumber](#) stores the Chemical Abstracts Service registry number.

## Example:

The CAS number of cocaine (CAS 50-36-2) serves as an index into the NIST Library. The NIST Library contains substantial about of compound information:

## Search Options [top](#)

### General Searches

- [Formula](#)
- [Name](#)
- [CAS registry number](#)
- [Reaction](#)
- [Author](#)
- [Structure](#)

### Physical Property Based Searches

- [Ion energetics properties](#)
- [Vibrational and electronic energies](#)
- [Molecular weight](#)

A CAS registry number is separated by hyphens into three parts, the first consisting of up to six digits, the second consisting of two digits, and the third consisting of a single digit serving as a check digit. The numbers are assigned in increasing order and do not have any inherent meaning. The checksum is calculated by taking the last digit times 1, the next digit times 2, the next digit times 3 etc., adding all these up and computing the sum modulo 10.

CAS values with a prefix of 1000 or 990 are not actual Chemical Abstract Service numbers but a value assigned by the library creator when the chemical has not yet been assigned a number by the Chemical Abstract Service at the time the library was created.

## Example:

The CAS number of water is 7732-18-5: the checksum is calculated as  $(8 \times 1 + 1 \times 2 + 2 \times 3 + 3 \times 4 + 7 \times 5 + 7 \times 6) = 105$ ;  $105 \bmod 10 = 5$ .

## CCISTDResponseRatioLimitHigh

[CCISTDResponseRatioLimitHigh](#) represents the high limit for the continuing calibration ISTD response ratio involved in the [CCISTDResponseRatio](#) outlier.

## CCISTDResponseRatioLimitLow

[CCISTDResponseRatioLimitLow](#) represents the low limit for the continuing calibration ISTD response ratio involved in the [CCISTDResponseRatio](#) outlier.

## CCResponseRatioLimitHigh

[CCResponseRatioLimitHigh](#) represents the high limit for the continuing calibration response ratio involved in the [CCResponseRatio](#) outlier.

## CCResponseRatioLimitLow

[CCResponseRatioLimitLow](#) represents the low limit for the continuing calibration response ratio involved in the [CCResponseRatio](#) outlier.

## CellAcceleratorVoltage

[CellAcceleratorVoltage](#) represents a meta data from LCQQQ acquisition.

## CoelutionScoreLimit

[CoelutionScoreLimit](#) represents the outlier limit for the Coelution Score outlier.

## CollisionEnergy

[CollisionEnergy](#) represents the amount of collision-induced dissociation (CID) occurring in the triple (QQQ) collision cell. CID is a mechanism to fragment molecular ions in the gas phase. The molecular ions are accelerated by this electrical potential to high kinetic energy in the vacuum of a mass spectrometer and to collide in the higher pressure collision cell with neutral gas molecules (nitrogen). In the collision some of the kinetic energy is converted into internal

energy which results in bond breakage and the fragmentation of the molecular ion into smaller fragments.

## CollisionEnergyDelta

[CollisionEnergyDelta](#) defines the one-sided extend of the chromatograms/spectra extraction range of the CollisionEnergy. If this value is set, the actual extraction range of chromatograms and spectra is given by the following formula:

$$\text{CE range} = [\text{CollisionEnergy} - \text{CollisionEnergyDelta}, \text{CollisionEnergy} + \text{CollisionEnergyDelta}]$$

The quantifier and each of the qualifier ions can be assigned independent CE extraction ranges.

## ColumnVoidTime

[ColumnVoidTime](#) is the retention time of unretained compound.

## CompoundApproved

[CompoundApproved](#) records the user's decision on the status of the compound in a sample. For example, the user sets the CompoundApproved status to True, meaning the compound in this sample is considered approved.

CompoundApproved is initialized to `NULL` and editable by the user in Batch-at-a-Glance.

## CompoundName

[CompoundName](#) represents a human-readable, non-unique identifier for a TargetCompound row. Typically it will be a standard structural or generic chemical name for the compound.

# CompoundGroup

[CompoundGroup](#) allows a classification of a particular compound with other similarly recorded compounds.

This association of individual compounds enables grouping of compounds as a unit. For example, the chemical group of PCBs (polychlorinated biphenyls) is composed of a numerous compounds (congeners) which make up total PCBs. Each individual compound makes a percent contribution to the total PCBs in the mixture.

# CompoundMath

[CompoundMath](#) allows aggregation of compounds in the same CompoundGroup for the math calculations in the following table.

Enum Name	UI Name
ResponseSum	Response Sum
ResponseAverage	Response Average
ResponseRatio	Response Ratio
ConcentrationSum	Concentration Sum
ConcentrationAverage	Concentration Average
ConcentrationRatio	Concentration Ratio
TPHResponseSubtraction	TPH Subtraction

Setup:

## 1) Set up individual compounds

In the "CompoundGroup" column, compounds aggregated together need to be assigned to the same group. Sublist is supported in Compound Group Math, i.e., if a compound is assigned in multiple groups (separated by comma), all assigned groups will contain the contribution from this compound.

For ResponseRatio and ConcentrationRatio, "\_D" or "\_N" need to be appended to the compound group name to indicate denominator and numerator.

## 2) Set up aggregate compounds

Add a new compound as the aggregate compound, and assign a single "Compound Group". Sublist should only be used for the individual compound. In the TargetCompound/CompoundGroupMath column, select a value from the pulldown menu {ConcentrationSum, ConcentrationAverage, ConcentrationRatio, ResponseSum, ResponseAverage, ResponseRatio}.



If a compound is assigned "ResponseSum" or "ResponseAverage", the responses of all the individual compounds from the same compound group will be aggregated (summed or averaged), for both calibration and quantitation.

If a compound is assigned "ConcentrationSum" or "ConcentrationAverage", the calculated concentrations and final concentrations will be aggregated (summed or averaged). Responses and Calibration curves are meaningless for concentration aggregated compounds.

- 3) For TPH Subtraction, no compound group set up is needed, only "TPH Subtraction" needs to be selected for the TPH compounds. The algorithm will find the surrogate/ISTD compounds that are within TPH integration range and subtract responses of them from TPH compound.

Note:

- 1) If an individual participating compound is manually integrated, peak results of a corresponding aggregate compound will be updated. For response-based compound math, area/height/targetResponse will be updated, as well as concentrations. For concentration-based compound math, only concentrations will be updated. The "MI" (manual integration) flag will be checked too.
- 2) Manual integration of the aggregate compound is cleared only if manual integration is cleared for all compounds in the same group.
- 3) If the aggregate compound is set as Response Average or Concentration Average, and the individual participating compound is zero peaked, the zero peaked compound will not contribute to the average.
- 4) Relative ISTD is not supported with Compound Math.

## CompoundType

[CompoundType](#) represents a human-readable classification tag relating to the user the function of this compound within the chemical analysis represented by this Quantitation DataSet class instance. Possible values (in English) would include "Target", "ISTD", "Surrogate", and "Matrix Spike". This string is subject to localization in other supported languages.

Enum Name	UI Name	XPath expression
Target	Target	*//CompoundType[.='Target']
ISTD	ISTD	*//CompoundType[.='ISTD']
Surrogate	Surrogate	*//CompoundType[.='Surrogate']
MatrixSpike	Matrix Spike	*//CompoundType[.='MatrixSpike']

## ConcentrationUnits

[ConcentrationUnits](#) represents a human readable string which defines the units of measurement for all measured and nominal concentration values associated with the quantitation of this TargetCompound row.

Default value is "µg/ml".

## CurveFit

[CurveFit](#) is a human-readable string that represents the curve-fitting mathematical model applied to the set of (response, concentration) calibration data points associated with any chemical analysis experiment run for the represented target compound against this Quantitation DataSet class instance. In English, its possible values include "Linear", "Quadratic", "Power", "First order ln", "Second order ln", and "Average of Response Factors".

This string is subject to localization in other supported languages.

## CurveFitFormula

[CurveFitFormula](#) represents an equation of the curve-fit model applied to the calibration data for this compound.

### Example:

The equation:  $y = 0.0603 x^2 + 0.3520 * x + 00033$

CurveFitFormula represents a quadratic calibration curve fit, where y is the response and x is the concentration.

## CurveFitLimitHigh

[CurveFitLimitHigh](#) represents the highest concentration in the set of enabled calibration points for this compound. CurveFitLimitHigh is computed internally by the system and is used to evaluate the Calibration Range outlier condition. QC points and Continuing Calibration points are ignored when calculating CurveFitLimitHigh.

## CurveFitLimitLow

[CurveFitLimitLow](#) represents the lowest concentration in the set of enabled calibration points for this compound. CurveFitLimitLow is computed internally by the system and is used to evaluate the Calibration Range outlier condition. QC points and Continuing Calibration points are ignored when calculating CurveFitLimitLow.

## CurveFitMinimumR

[CurveFitMinimumR](#) represents the limit for the Curve Fit R outlier. [OutlierCurveFitR](#) is set to Low if the value of CurveFitR for this compound is less than CurveFitMinimumR.

## CurveFitMinimumR2

[CurveFitMinimumR2](#) represents the limit for the Curve Fit R2 outlier. [OutlierMinimumCurveFitR2](#) is set to Low if the value of CurveFitR2 for this compound is less than CurveFitMinimumR2.

## CurveFitOrigin

[CurveFitOrigin](#) is a human-readable string that represents the treatment of the point (0, 0) with respect to the set of (response, concentration) calibration data points regressed using the curve-fitting mathematical model represented by the CurveFit column. In English, its possible values include "Ignore", "Include", and "Force". This string is subject to localization in other supported languages. To Ignore the point (0, 0) means that no (0, 0) point is added to the set of calibration data points. To Include the point (0, 0) means that the (0, 0) point is added to the set of calibration data points if it does not exist already. To Force the point (0, 0) means that curve-fitting mathematical model represented by the CurveFit column is further constrained such that the fitting equation/curve must pass through the point (0, 0). Note that the Force and Include options are not meaningful for some Power and Logarithmic curve-fitting models.

In addition, CurveFitOrigin includes the choice "Blank Offset". In this case, the following curve fit formula applies:

$$y = ax + \textit{BlankOffset}$$

where blankOffset is the BlankResponseOffset column, which is the average target response of "Blank" samples in the batch. The value is subtracted from each calibration levels, and the Force Origin calibration curve is applied to calculate "a" in " $y = ax + \textit{BlankOffset}$ "

Enum Name	UI Name	XPath expression
originIgnore	Ignore	*//CurveFitOrigin[.='originIgnore']
originInclude	Include	*//CurveFitOrigin[.='originInclude']
originForce	Force	*//CurveFitOrigin[.='originForce']

originBlankOffset	Blank Offset	<code>*//CurveFitOrigin[.='originBlankOffset']</code>
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## CurveFitR

[CurveFitR](#) is a measure of the linear correlation between two variables  $X$  and  $Y$ . It has a value between +1 and -1, where 1 is total positive linear correlation, 0 is no linear correlation, and -1 is total negative linear correlation. The calculation is:

$$R_{xy} = \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^n (x_i - \bar{x})^2} \sqrt{\sum_{i=1}^n (y_i - \bar{y})^2}}$$

## CurveFitR2

[CurveFitR2](#) is a measure of the quality of the calibration curve fit, known as  $R^2$  or the coefficient of determination. It is a number between 0 and 1 such that a perfect fit (for example, all calibration points falling on a straight line for linear fit) corresponds to  $R^2 = 1$ . [CurveFitR2](#) is subject to the Curve Fit  $R^2$  outlier condition.

## CurveFitStatus

[CurveFitStatus](#) is a human-readable string that represents the success or error status of the calibration curve fit and its subsequent use in converting the target response to compound concentration. In English, its possible values include "Success", "NotEnoughDataPoints", "NotConverged", "ResponseOutOfRange", and "UnknownError". This string is subject to localization in other supported languages. The value "NotEnoughDataPoints" indicates that the number of calibration points is insufficient for the curve fit of the specified type. The value "NotConverged" indicates a poor match between the set of calibration data points and the selected curve fit type. The value "ResponseOutOfRange" indicates that the response value cannot be converted to a concentration value on the calibration curve. This can occur for a quadratic curve fit, for example, if the target response is below the bottom or above the top of the parabola. The value "UnknownError" corresponds to an internal application error.

Enum Name	UI Name	XPath expression
Success	Success	*//CurveFitStatus[.='Success']
NotEnoughDataPoints	NotEnoughDataPoints	*//CurveFitStatus[.='NotEnoughDataPoints']
NotConverged	NotConverged	*//CurveFitStatus[.='NotConverged']
ResponseOutOfRange	ResponseOutOfRange	*//CurveFitStatus[.='ResponseOutOfRange']
UnknownError	UnknownError	*//CurveFitStatus[.='UnknownError']

## CurveFitWeight

[CurveFitWeight](#) is a human-readable string that represents the weighting function applied to the various members of the set of (response, concentration) calibration data points regressed using the curve-fitting mathematical model represented by the CurveFit column. As the weighting function is applied to each data point in the regression set, it affects the contribution of each individual data point to the ultimate determination of the regression equation. In English, its possible values include "None", "1/x", "1/x^2", "1/y", and "1/y^2". This string (in particular for the case of "None") is subject to localization in other supported languages. X or Y members of data points are weighted as indicated by the CurveFitWeight string. In the case of "None", a weighting factor of unity is applied to all X and Y components of all calibration data points.

In addition, the CurveFit choice includes "1/SD^2". The weight assigned to each calibration point is one over the variance (standard deviation squared) of the responses of the replicate calibration points at the same level as that point. In this case, if any of the levels have no replicates, the curve fit fails.

When the CurveFitOrigin is set to "originInclude" and CurveFitWeight is set to 1/x, 1/x^2, 1/y or 1/y^2, origin gets a weight of zero.

Enum Name	UI Name	XPath expression
weightEqual	None	*//CurveFitWeight[.='weightEqual']
weightOneOverX	1/x	*//CurveFitWeight[.='weightOneOverX']
weightOneOverXSquared	1/x^2	*//CurveFitWeight[.='weightOneOverXSquared']
weightOneOverY	1/y	*//CurveFitWeight[.='weightOneOverY']
weightOneOverYSquared	1/y^2	*//CurveFitWeight[.='weightOneOverYSquared']
weightLog	Log	*//CurveFitWeight[.='weightLog']
weightOneOverSDSquared	1/SD^2	*//CurveFitWeight[.='weightOneOverSDSquared']

## DilutionHighestConcentration

[DilutionHighestConcentration](#) represents the highest concentration in the applied DilutionPattern.

## DilutionPattern

[DilutionPattern](#) represents a scheme or series used to create the concentration standards. A serial dilution pattern is typically accomplished by starting with the DilutionHighestConcentration and repeatedly applying the dilution pattern.

### Examples:

A pattern such as 1:10 means 1 part sample diluted with 9 parts liquid. For an example of the 1:2 dilution pattern, see table below.

Standard Number	(pg/ml)	( $\mu$ l)	Diluent ( $\mu$ l) Volume
1	4000	50 $\mu$ l	950 $\mu$ l
2	2000	500 $\mu$ l of #1	500 $\mu$ l
3	1000	500 $\mu$ l of #2	500 $\mu$ l
4	500	500 $\mu$ l of #3	500 $\mu$ l
5	250	500 $\mu$ l of #4	500 $\mu$ l

DilutionPattern format is not limited to a single dilution factor.

Two more examples help illustrate the DilutionPattern and its effect on the serial dilution sequence:

- 1) DilutionPattern of 1 : 2 : 2.5 with DilutionHighestConcentration = 500 yields the following series: 500, 250, 100, 50, 20, 10, 4, 2, 0.8, 0.4, 0.16, 0.08...
- 2) DilutionPattern of 1 : 2 : 2.5 : 4 with DilutionHighestConcentration = 500 yields the following series: 500, 250, 100, 25, 12.5, 5.0, 1.25, 0.625, 0.25, 0.0625...

## DynamicTargetCompoundID

[DynamicTargetCompoundID](#) represents a forward pointer from the user-defined compound to the dynamic target. Null if there are no dynamic targets for this compound. Equal to the CompoundID of the dynamic target compound actually used for quantitation in the current sample at runtime.

## DynamicTargetRank

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[DynamicTargetRank](#) represents a unique integer for each user-defined compound ID.

## ExpectedConcentration

[ExpectedConcentration](#) represents a concentration measurement expressed in units of ConcentrationUnits. This value defines the nominal concentration for this compound in the sample represented by SampleID.

## FragmentorVoltage

[FragmentorVoltage](#) represents the acquisition parameter that controls the acceleration of the ions from the source into the rest of the mass spectrometer (mass analyzer and detection).

## FragmentorVoltageDelta

[FragmentorVoltageDelta](#) defines the one-sided extent of the chromatograms/spectra extraction range of the FragmentorVoltage. If this value is set, the actual extraction range of chromatograms and spectra is given by the following formula:

$$\text{FV range} = [\text{FragmentorVoltage} - \text{FragmentorVoltageDelta}, \text{FragmentorVoltage} + \text{FragmentorVoltageDelta}]$$

In this formula, the bottom of the FV range is constrained to be non-negative. The quantifier and each of the qualifier ions can be assigned independent FV extraction ranges.

## FullWidthHalfMaximumLimitHigh

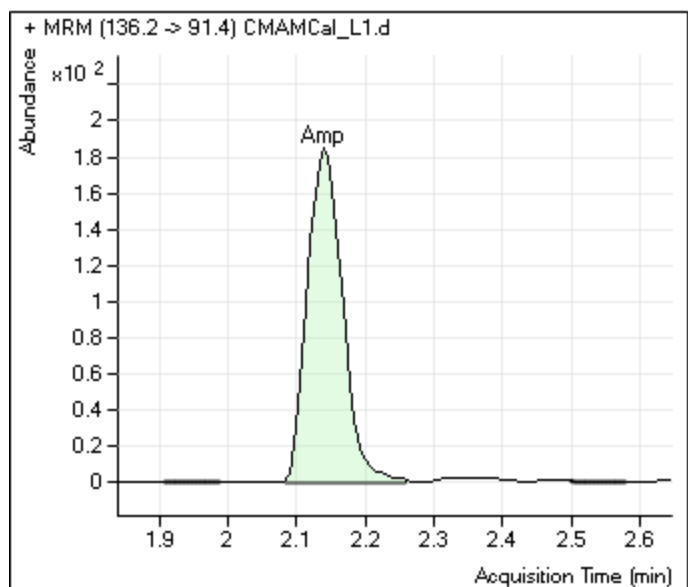
[FullWidthHalfMaximumLimitHigh](#) represents the higher limit for the full width half maximum outlier. [OutlierFullWidthHalfMaximum](#) is set to Low if the calculated [FullWidthHalfMaximum](#) value of the primary peak is less than the [FullWidthHalfMaximumLimitLow](#).

## FullWidthHalfMaximumLimitLow

[FullWidthHalfMaximumLimitLow](#) represents the lower limit for the full width half maximum outlier. [OutlierFullWidthHalfMaximum](#) is set to Low if the calculated [FullWidthHalfMaximum](#) value of the primary peak is less than the [FullWidthHalfMaximumLimitLow](#).

## GraphicPeakChromatogram

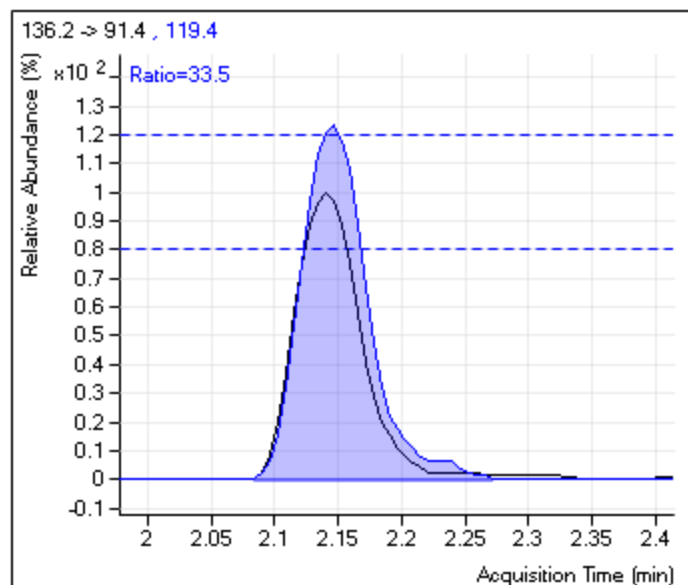
[GraphicPeakChromatogram](#) represents a relative path and filename to a graphic (.emf) file used in reporting.



Graphic 2: File reference to graphic.

## GraphicPeakQualifiers

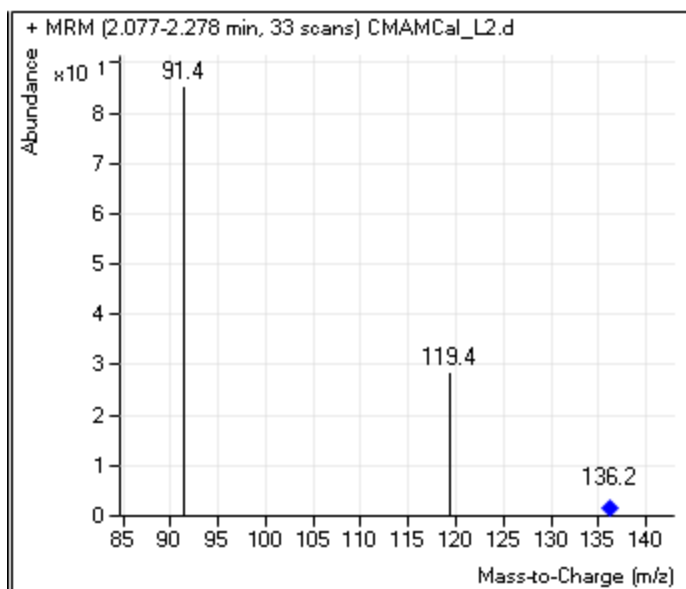
[GraphicPeakQualifiers](#) represents a relative path and filename to a graphic (.emf) file used in reporting.



Graphic 3: File reference to graphic.

## GraphicPeakSpectrum

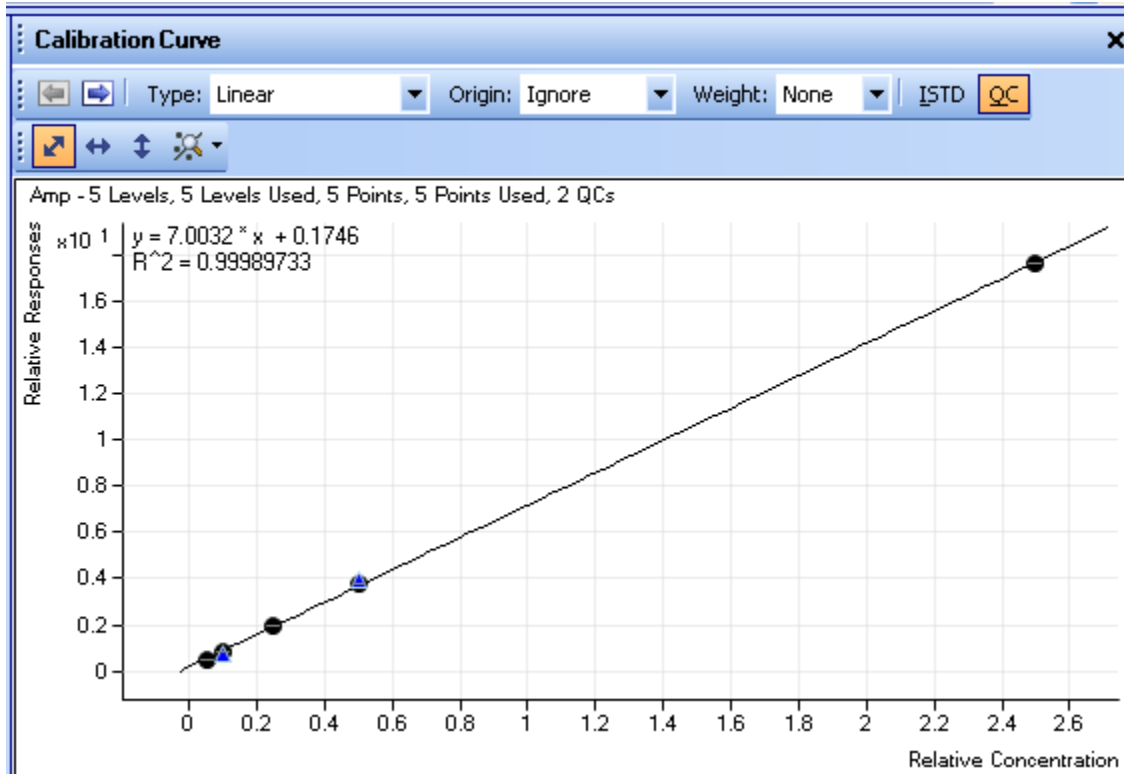
[GraphicPeakSpectrum](#) represents a relative path and filename to a graphic (.emf) file used in reporting.



**Graphic 4: File reference to graphic.**

# GraphicTargetCompoundCalibration

[GraphicTargetCompoundCalibration](#) represents a relative path and filename to a graphic (.emf) file used in reporting.



Graphic 5: File reference to Calibration graphic.

## ID

[ID](#) represents the user index for a compound.

## InstrumentName

[InstrumentName](#) represents the name of a particular instrument. Typically, InstrumentName is set by the sample information entered during acquisition.

## InstrumentType

[InstrumentType](#) is defaulted to QQQ. As a rule, only one type of instrument comprises a particular batch.

Enum Name	UI Name	XPath expression
QQQ	QQQ	*//InstrumentType[.='QQQ']
QTOF	QTOF	*//InstrumentType[.='QTOF']
TOF	TOF	*//InstrumentType[.='TOF']
GCMS	GCMS	*//InstrumentType[.='GCMS']
LCMS	LCMS	*//InstrumentType[.='LCMS']
Unspecified		

## IntegrationParameters

[IntegrationParameters](#) represents a collection of parameters that modulate the behavior of the General integration algorithm brought to bear on the signal indicated by this TargetCompound row. The default value for IntegrationParameters is NULL. Wherever this column is NULL, signal integration proceeds assuming the default integration settings in the context of the integrator used.

## IntegrationParametersModified

[IntegrationParametersModified](#) is true when the integration parameters for a compound is modified at the sample level.

# Integrator

[Integrator](#) represents the choice of Integrator algorithm from the following:

- Agile Integrator
- MS-MS Integrator
- General Integrator
- MS-MS (GC)
- Universal
- Spectral Summer

The MS-MS Integrator is especially applicable to the signal characteristics of the triple mass spectrometer.

Enum Name	UI Name	XPath expression
Agile	Agile	*//Integrator[.='Agile']
RTE	General	*//Integrator[.='RTE']
AutoMagic	MS-MS	*//Integrator[.='AutoMagic']
Genie	Universal	*//Integrator[.='Genie']
AutoMagic2	MS	*//Integrator[.='AutoMagic2']
SpectralSummer	Spectral Summer	*//Integrator[.='SpectralSummer']

General integrator was formerly called the RTE integrator.

Universal integrator was formerly called the GC-MS Genie integrator.

# IonPolarity

[IonPolarity](#) represents an acquisition parameter that records the polarity of the ions focused with voltages applied to a lens system located between the source and the analyzer.

Enum Name	UI Name	XPath expression	Summary
Positive	Positive	*//IonPolarity[.='Positive']	Positive ion polarity
Negative	Negative	*//IonPolarity[.='Negative']	Negative ion polarity

Unassigned	Unassigned	*//IonPolarity[.='Unassigned']	Unknown ion polarity
Mixed	Mixed	*//IonPolarity[.='Mixed']	Contains both positive and negative ion polarity data

## IonSource

[IonSource](#) represents the acquisition parameter that record the type of source used in the mass spectrometer including:

For example, with the triple (LC-QQQ):

- ESI: Electro Spray Ionization
- APCI: Atmospheric Pressure Chemical Ionization
- MultiMode (both)

## ISTDCompoundID

[ISTDCompoundID](#) represents a link to another TargetCompound row. The TargetCompound row so linked implies the internal standard compound with which is associated the target compound represented by this TargetCompound row. If the value of ISTDCompoundID is -1, then the target compound represented by this TargetCompound row is not associated with an internal standard.

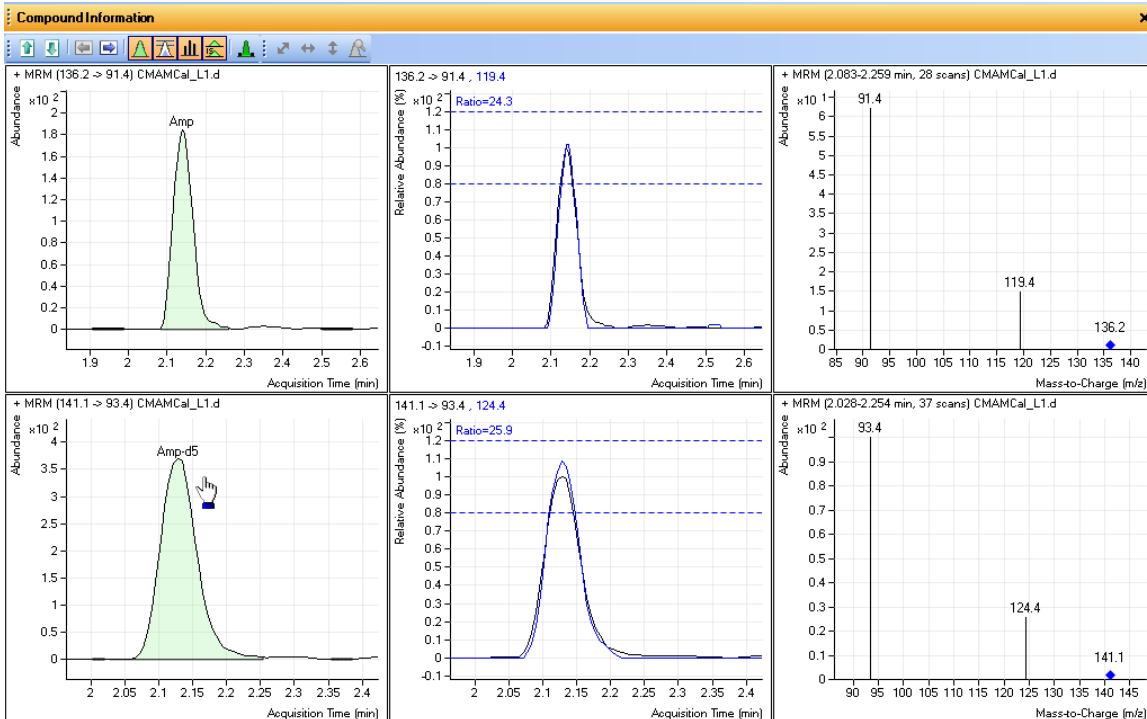
## ISTDConcentration

[ISTDConcentration](#) represents a concentration measurement expressed in units of ConcentrationUnits. This value indicates the nominal concentration of internal standard in any Sample under analysis versus this Quantitation DataSet class instance. This value is only meaningful if this TargetCompound row has a value of true for its ISTDFlag member.



# ISTDFlag

[ISTDFlag](#) represents the value true if and only if this TargetCompound row represents an internal standard compound.



**ISTD 1: Relationship of Target to its associated ISTD (internal standard).**

## ISTDResponseLimitHigh

[ISTDResponseLimitHigh](#) represents the upper limit criteria for the outlier [OutlierISTDResponse](#).

## ISTDResponseLimitLow

[ISTDResponseLimitLow](#) represents the lower limit criteria for the outlier [OutlierISTDResponse](#).

## ISTDResponseMaximumPercentDeviation

[ISTDResponseMaximumPercentDeviation](#) represents the upper limit criteria for the outlier [OutlierISTDResponsePercentDeviation](#).

## ISTDResponseMinimumPercentDeviation

[ISTDResponseMinimumPercentDeviation](#) represents the lower limit criteria for the outlier  
OutlierISTDResponsePercentDeviation.

# KEGGID

[KEGGID](#) represents an identifier in KEGG (Kyoto Encyclopedia of Genes and Genomes) database.

## LeftRetentionTimeDelta

[LeftRetentionTimeDelta](#) represents a value expressed in units of minutes or percent of nominal RetentionTime, as indicated by RetentionTimeDeltaUnits. It defines the offset used to determine the lower bound for the retention-time window for signals which are extracted in support of quantitating the chemical compound indicated by this TargetCompound row.

### Example:

RetentionTime has a value of 5 minutes. LeftRetentionTimeDelta has a value of 0.1 and RetentionTimeDeltaUnits has a value of 0 for Minutes. Then the lower bound on the extraction window is  $5 - 0.1$  or 4.9 minutes. On the other hand if RetentionTimeDeltaUnits is 1 for Percent and LeftRetentionTimeDelta is 20, then the lower bound on the extraction window is  $5 - 20\% * 5 = 4$  minutes. Default value is 1 minutes.

## LibraryMatchScore

[LibraryMatchScore](#) records the measure of the correlation between the deconvoluted peak's spectrum and the standard spectrum from the library searched.

LibraryMatchScore is an indicator of the quality of the library match and low LibraryMatchScores should be investigated and identify of the compound identification confirmed.

The measure of 100 means a perfect match.

## LibraryMatchScoreMinimum

[LibraryMatchScoreMinimum](#) represents the lower limit for the Library Match Score outlier. OutlierLibraryMatchScore is set to Low if the LibraryMatchScore of this compound is less than LibraryMatchScoreMinimum.

## LibraryRetentionIndex

[LibraryRetentionIndex](#) records the retention index determined from the library search.

LibraryRetentionIndex requires the compound is perceived using a retention time calibration (RT CAL).

The RT CAL information holds the relationship between the retention time (RT) and retention index (RI). Using the RI information in the library along with the RT CAL mapping enables a user to search the library with RIs.

## LibraryRetentionTime

[LibraryRetentionTime](#) records the retention time from the library search.

LibraryRetentionTime is the expected RT stored in the library. Comparing the LibraryRetentionTime with the actual RT is useful in evaluating the compound's identification.

## LimitOfDetection

[LimitOfDetection](#) (LOD) represents the lowest quantity of a substance that can be distinguished from the absence of that substance (a *blank value*). Typically, the blank value plus three standard deviations is established as the LOD.

## LimitOfQuantitation

[LimitOfQuantitation](#) (LOQ) represents the concentration at which quantitative results can be reported with a high degree of confidence. Typically, the LOQ is determined by an empirical approach, consisting of measuring progressively more dilute concentrations of analyte.

## LinearResponseRangeMax

[LinearResponseRangeMax](#) represents high end of the range of area responses over which the quantifier response is linear vs. concentration.

## LinearResponseRangeMin

[LinearResponseRangeMin](#) represents low end of the range of area responses over which the quantifier response is linear vs. concentration.

## MassAccuracyLimit

[MassAccuracyLimit](#) represents the limit for the Mass Accuracy outlier. [OutlierMassAccuracy](#) is set to High if the [MassAccuracy](#) exceeds MassAccuracyLimit. [OutlierMassAccuracy](#) is set to Low if the [MassAccuracy](#) is less than negative MassAccuracyLimit.

## MassMatchScoreMinimum

[MassMatchScoreMinimum](#) represents the lower limit for the Mass Match Score outlier. OutlierMassMatchScore is set to Low if the MassMatchScore of this compound is less than MassMatchScoreMinimum.

## MatrixAConcentrationLimitHigh

[MatrixAConcentrationLimitHigh](#) represents the upper limit for the Matrix Spike outlier for type-A matrix compounds. [OutlierMatrixSpikeOutOfLimits](#) is set to High if the FinalConcentration of a type-A matrix compound exceeds MatrixAConcentrationLimitHigh.

## MatrixAConcentrationLimitLow

[MatrixAConcentrationLimitLow](#) represents the lower limit for the Matrix Spike outlier for type-A matrix compounds. [OutlierMatrixSpikeOutOfLimits](#) is set to Low if the FinalConcentration of a type-A matrix compound is less than MatrixAConcentrationLimitLow.

## MatrixBConcentrationLimitHigh

[MatrixBConcentrationLimitHigh](#) represents the upper limit for the Matrix Spike outlier for type-B matrix compounds. [OutlierMatrixSpikeOutOfLimits](#) is set to High if the FinalConcentration of a type-B matrix compound exceeds MatrixBConcentrationLimitHigh.

## MatrixBConcentrationLimitLow

[MatrixBConcentrationLimitLow](#) represents the lower limit for the Matrix Spike outlier for type-B matrix compounds. [OutlierMatrixSpikeOutOfLimits](#) is set to Low if the FinalConcentration of a type-B matrix compound is less than MatrixBConcentrationLimitLow.

## MatrixSpikeConcentration

[MatrixSpikeConcentration](#) represents the expected concentration of a matrix spike compound of either type A or type B. MatrixSpikeConcentration is used to calculate the matrix spike percent recovery.

## MatrixSpikePercentRecoveryMaximum

[MatrixSpikePercentRecoveryMaximum](#) represents the upper limit for the Matrix Spike Percent Recovery outlier. [OutlierMatrixSpikePercentRecovery](#) is set to High if the percent recovery of this matrix compound exceeds MatrixSpikePercentRecoveryMaximum.

## MatrixSpikePercentRecoveryMinimum

[MatrixSpikePercentRecoveryMinimum](#) represents the lower limit for the Matrix Spike Percent Recovery outlier. [OutlierMatrixSpikePercentRecovery](#) is set to Low if the percent recovery of this matrix compound is less than MatrixSpikePercentRecoveryMinimum.

## MatrixSpikeMaximumPercentDeviation

[MatrixSpikeMaximumPercentDeviation](#) represents the limit for the Matrix Spike Percent Difference outlier. [OutlierMatrixSpikeOutsidePercentDeviation](#) is set to High if the percent difference between the concentrations for a given matrix compound in the Matrix sample and in the MatrixDup sample exceeds MatrixSpikeMaximumPercentDeviation.

## MatrixSpikeBMaximumPercentDeviation

[MatrixSpikeBMaximumPercentDeviation](#) represents the limit for the Matrix Spike Percent Difference outlier for type B matrix spike compound. [OutlierMatrixSpikeOutsidePercentDeviation](#) is set to High if the percent difference between the concentrations for a given matrix compound in the Matrix sample and in the MatrixDup sample exceeds MatrixSpikeMaximumPercentDeviation.

## MatrixTypeOverride

[MatrixTypeOverride](#) is an xml string that can record target compound columns on a per sample per compound base based on the Matrix Type match. It's used together with [MatrixType](#) to define different outlier limits for different Matrix.

## MaximumAverageResponseFactorRSD

[MaximumAverageResponseFactorRSD](#) represents the limit for the Average Response Factor RSD outlier. [AverageOutlierResponseFactorRSD](#) is set to High if AverageResponseFactorRSD for this compound is greater than MaximumAverageResponseFactorRSD.

## MaximumBlankConcentration

[MaximumBlankConcentration](#) represents the limit for the Blank Concentration outlier. OutlierBlankConcentrationOutsideLimit is set to High if the CalculatedConcentration for this compound in a blank sample exceeds MaximumBlankConcentration.

## MaximumBlankResponse

[MaximumBlankResponse](#) represents the limit for the Blank Response outlier. OutlierBlankResponseOutsideLimit is set to High if the Response for this compound in a blank or double-blank sample exceeds MaximumBlankResponse. OutlierBlankResponseOutsideLimit is also set to High if the ISTD Response in a double-blank sample exceeds MaximumBlankResponse.

## MaximumCCResponseFactorDeviation

[MaximumCCResponseFactorDeviation](#) represents the maximum limit for the [CCAverageResponseFactor](#) outlier calculation.



## MaximumNumberOfHits

[MaximumNumberOfHits](#) is an integer which places an upper bound on the number of peaks that will be stored as linked Peak rows and thus be candidates for quantitation. The default value for MaximumNumberOfHits is nine.

## MaximumPercentResidual

[MaximumPercentResidual](#) represents the largest percent residual of all enabled calibration points for this compound. The percent residual of a calibration point is defined as the percent difference between the actual response value and the result of evaluating the curve fit formula at the calibration point's concentration.

## Method Detection Limit

[MethodDetectionLimit](#) (MDL) represents the minimum concentration of a substance that can be measured and reported with 99% confidence that the analyte concentration is greater than zero, and is determined from analysis of a sample in a given matrix containing the analyte.

## MinimumAssignedNoise

[MinimumAssignedNoise](#) defines a value, in counts, of the noise that is assigned to a peak if no noise regions can be found or if the computed noise over all noise regions is zero.

## MinimumAverageResponseFactor

[MinimumAverageResponseFactor](#) represents the limit for the Average Response Factor outlier. [OutlierAverageResponseFactor](#) is set to Low if AverageResponseFactor for this compound is less than MinimumAverageResponseFactor.

## MinimumCCRelativeResponseFactor

[MinimumCCRelativeResponseFactor](#) represents the minimum limit for the CC Relative Response Factor outlier involved in the [OutlierCCRelativeResponseFactor](#) outlier.

## MinimumPercentPurity

[MinimumPercentPurity](#) represents a lower limit for the Purity outlier. [OutlierPurity](#) is set to Low if the calculated Purity for this compound is less than MinimumPercentPurity.

## MinimumSignalToNoiseRatio

[MinimumSignalToNoiseRatio](#) represents the limit for the Signal to Noise Ratio outlier. [OutlierSignalToNoiseRatioBelowLimit](#) is set to Low if SignalToNoise for this compound's primary peak is less than [MinimumSignalToNoiseRatio](#).

## MolecularFormula

[MolecularFormula](#) store the compound's composition of atoms.

## Multiplier

[Multiplier](#) represents a conversion factor that is used to obtain the [FinalConcentration](#) from the [CalculatedConcentration](#):

$$\text{FinalConcentration} = \text{CalculatedConcentration} \times \text{Multiplier}$$

The value of the Multiplier is determined by the values of [Dilution](#), [SampleAmount](#), and [TotalSampleAmount](#):

$$\text{Multiplier} = \text{DilutionMultiplier} \times \text{SampleAmountMultiplier}$$

Here:

$$\text{DilutionMultiplier} = \text{Dilution}, \text{ if defined; otherwise } 1$$

$$\text{SampleAmountMultiplier} = \text{TotalSampleAmount} \div \text{SampleAmount}, \text{ if both are defined; otherwise } 1$$

## MZ

[MZ](#) represent the mass to charge ratio. In the case of a tandem mass spectrometry experiment, MZ is a mass-to-charge measurement, in units of daltons per unit charge, of the ions selected by the final-quadrupole stage in a tandem mass spectrometer used to perform this experiment. In

the case of a single-quadrupole mass spectrometry experiment, MZ is a mass-to-charge measurement, in units of daltons per unit charge, of the ions selected by the single quadrupole stage in this experiment.

## MZAdditional

[MZAdditional](#) represent the additional MZs to be merged together with the quantifier MZ as a single chromatogram trace. Multiple MZs are separated by ";". Quantitation is based on the merged EIC if this field is defined.

## MZExtractionWindowFilterLeft

[MZExtractionWindowFilterLeft](#) represents the left side of the M/Z range for chromatogram extraction. The compound chromatograms are extracted over the M/Z range defined by

$$[MZ - MZExtractionWindowFilterLeft, MZ + MZExtractionWindowFilterRight]$$

## MZExtractionWindowFilterRight

[MZExtractionWindowFilterRight](#) represents the right side of the M/Z range for chromatogram extraction. The compound chromatograms are extracted over the M/Z range defined by

$$[MZ - MZExtractionWindowFilterLeft, MZ + MZExtractionWindowFilterRight]$$

# MZExtractionWindowUnits

[MZExtractionWindowUnits](#) represents the units used for [MZExtractionWindowFilterLeft](#) and [MZExtractionWindowFilterRight](#).

The units are the following:

- [Thomsons](#):

Thompson or m/z represents the physical quantity mass-to-charge ratio.

For example, the ion  $C_7H_7^{2+}$  an ion will be observed at 45.5 m/z

- PPM:

*Parts per million* ("ppm") denotes one particle of a given substance for every 999,999 other particles. One part in  $10^6$  — a precision of 0.0001%

The user can alternatively establish the mass extraction window value using ppm units.

$$\text{ppm} = 10^6 * \Delta m \text{ accuracy} / m_{\text{measured}}$$

For example, at the theoretical mass of 1000 and a measured mass of 999.9 boundary is designated as 100 ppm.

- Percent:

*Percent* represents the mass extraction window as a percentage of the theoretical mass.

Enum Name	UI Name	XPath expression
Thomsons	m/z	*//MZExtractionWindowUnits[.=' Thomsons ']
PPM	ppm	*//MZExtractionWindowUnits[.=' PPM' ]
Percent	Percent	*//MZExtractionWindowUnits[.=' Percent' ]

## MZScanRangeLow

[MZScanRangeLow](#) represents the bottom of the M/Z scan range. It is applicable only to those ScanType values that involve scanning the mass axis.

The mass range limits are typically NULL by default.

If both limits are defined, then the values must be consistent ( $\text{min} \leq \text{max}$ ).

Internally, MZScanRangeLow or MZScanRangeLow does not influence the spectral range actually extracted.

## MZScanRangeHigh

[MZScanRangeLow](#) represents the top of the M/Z scan range. It is applicable only to those ScanType values that involve scanning the mass axis.

The mass range limits are typically NULL by default.

If both limits are defined, then the values must be consistent ( $\text{min} \leq \text{max}$ ).

Internally, MZScanRangeLow or MZScanRangeLow does not influence the spectral range actually extracted.

## NeutralLossGain

[NeutralLossGain](#) represents the amount of neutral loss or gain, in M/Z units (daltons per unit charge). This column is only applicable to Neutral Loss and Neutral Gain scan types.

# NoiseAlgorithmType

[NoiseAlgorithmType](#) represents the choice of algorithm to use for calculating the [SignalToNoiseRatio](#) of a chromatogram peak. The following choices of NoiseAlgorithmType are available:

- Peak-to-Peak
- Peak-to-Peak from Drift
- ASTM (default)
- RMS
- Auto RMS

The noise calculation divides the chromatographic range into N “noise regions” that cover the entire range, excluding the peaks.

## Example:

If the chromatogram covers the retention time range of 0 to 3 minutes and there are two peaks, one extending from 1.3 to 1.7 minutes, the other extending from 2.2 minutes to 2.5 minutes, then there will be  $N = 3$  noise regions:

[0.0, 1.3], [1.7, 2.2], [2.5, 3.0]

Noise regions less than 3 points wide are eliminated. For the Peak-to-Peak and ASTM algorithms, the low and high abundance values are computed from the chromatogram over each noise region. Then, for the Peak-to-Peak algorithm, the noise is computed as the maximum high-low difference over all noise regions:

$$\text{Noise (Peak-to-Peak)} = \text{Max}( \text{High}_n - \text{Low}_n ) \text{ over } n = 1..N.$$

For the ASTM algorithm, the noise is computed as the average of the  $(\text{High}_n - \text{Low}_n)$  differences for each noise region:

$$\text{Noise (ASTM)} = \text{Average}( \text{High}_n - \text{Low}_n ) \text{ over } n = 1..N.$$

For RMS (root-mean-square) noise algorithm, the system computes the root-mean-square variation of abundance over each noise region and takes the maximum of the RMS values over all regions. The Peak-to-Peak from Drift algorithm uses linear regression to fit a drift line to each noise region and finds the difference of the maximum positive and maximum negative displacements from the regression line. The noise is then computed as the maximum displacement difference over all noise regions.

For Auto RMS, this algorithm works by moving a Noise region window across a defined noise region boundary and selecting the minimum noise value calculated from the Noise region window.

In order to calculate the signal-to-noise ratio, the chromatogram must be integrated first. A noise region boundary is defined with a **Start time** and **End time** in minutes. A Noise region window is moved across this noise region boundary one step at a time. At each step, at least three points must be inside the window in order to calculate the root-mean-square noise value. The smallest noise value computed is used. If the smallest noise value is 0, then the noise value is set to  $1/\sqrt{\text{bins}}$ . *Bins* is the number of points in the first Noise region window.

Enum Name	UI Name	XPath expression
PeaktoPeak	PeaktoPeak	*//NoiseAlgorithmType[.='PeaktoPeak']
PeaktoPeakDrift	PeaktoPeakDrift	*//NoiseAlgorithmType[.='PeaktoPeakDrift']
ASTM	ASTM	*//NoiseAlgorithmType[.='ASTM']
RMS	RMS	*//NoiseAlgorithmType[.='RMS']
AutoRMS	Auto RMS	*//NoiseAlgorithmType[.='AutoRMS']

## NoiseOfRawSignal

[NoiseOfRawSignal](#) represents the noise calculated for the extracted target signal. NoiseOfRawSignal is calculated regardless of whether an integrated peak exists or not. Different algorithms are supported as well as self-defined noise regions.

## NoiseReference

[NoiseReference](#) defines from what sample noise is calculated.

If "Sample" is selected for NoiseReference or if NoiseReference is null (blank), noise is calculated from the sample.

If "Blank" is selected for NoiseReference, noise is calculated using the noise in the last blank (sample type = Blank) acquired before the sample. For quantifiers: "NoiseOfRawSignal" of the quantifier peak in the blank sample is used. For qualifiers: Noise of the qualifier peak in the blank sample is used. If no qualifier peak is found in the blank sample, the qualifier EIC is extracted, and noise is calculated from the raw EIC.

The use of the blank's noise only applies to samples where sample type = "Sample", all other sample types will use the sample's noise.

## NoiseRegions

[NoiseRegions](#) defines a retention time window which is used to evaluate the noise for a particular chromatogram.

Assuming your chromatography is reproducible, you can pick a region in the chromatogram and the [SignalToNoiseRatio](#) calculation uses that region to evaluate the noise.

## NoiseStandardDeviationMultiplier

[NoiseStandardDeviationMultiplier](#) represents a multiplier that is applied to the noise value during the calculation of the SignalToNoiseRatio of a peak. For a given chromatogram, a NoiseStandardDeviationMultiplier value of 3 will result in a three-fold increase in the reported noise and therefore, a three-fold reduction in SignalToNoiseRatio. The default value of NoiseStandardDeviationMultiplier is 5.

## NonReferenceWindowOverride

[NonReferenceWindowOverride](#) is a compound level nonReferenceWindow setting, when it is not null, global nonReferenceWindow setting is overridden, and specified number is applied to this compound only.

## NumberOfVerifiedIonsLimit

[NumberOfVerifiedIonsLimit](#) is the outlier limit for the number of verified ions outlier. [OutlierNumberOfVerifiedIons](#) is set to Low if Number of verified ions for this compound is less than NumberOfVerifiedIonsLimit.

## OutlierAlternativePeak

[OutlierAlternativePeak](#) stores the flag resulting from the [Alternative Peak outlier](#) condition evaluation. If [enabled by default](#) or by applying Outlier Setup, an associated column is highlighted.

## OutlierAverageResponseFactor



[OutlierAverageResponseFactor](#) stores the flag resulting from the [Average Response Factor outlier](#) condition evaluation. If [enabled by default](#) or by applying Outlier Setup, an associated column is highlighted.

## OutlierAverageResponseFactorRSD

[OutlierAverageResponseFactorRSD](#) stores the flag resulting from the [Average Response Factor RSD outlier](#) condition evaluation. If [enabled by default](#) or by applying Outlier Setup, an associated column is highlighted.

## OutlierBlankResponseOutsideLimit

[OutlierBlankResponseOutsideLimit](#) stores the flag resulting from the Blank Response [outlier condition evaluation](#). If [enabled by default](#) or by applying Outlier Setup, an associated column is highlighted. See [Outlier Details](#).

## OutlierCCAverageResponseFactor

[OutlierCCAverageResponseFactor](#) stores the flag resulting from the [Average CC Response Factor outlier](#) condition evaluation. If [enabled by default](#) or by applying Outlier Setup, an associated column is highlighted.

## OutlierCCRelativeResponseFactor

[OutlierCCRelativeResponseFactor](#) stores the flag resulting from the [Average CC Relative Response Factor outlier](#) condition evaluation. If [enabled by default](#) or by applying Outlier Setup, an associated column is highlighted.

## OutlierCustomCalculation

[OutlierCustomCalculation](#) stores the flag resulting from the [User Custom Calculation](#) condition evaluation. If [enabled by default](#) or by applying Outlier Setup, an associated column is highlighted.

## OutlierCurveFitR

[OutlierCurveFitR](#) stores the flag resulting from the [Curve Fit R outlier](#) condition evaluation. If [enabled by default](#) or by applying Outlier Setup, an associated column is highlighted.

## OutlierMethodDetectionLimit

[OutlierMethodDetectionLimit](#) stores the flag resulting from the Method Detection Limit outlier condition evaluation. If [enabled by default](#) or by applying Outlier Setup, an associated column is highlighted.

## OutlierMinimumCurveFitR2

[OutlierMinimumCurveFitR2](#) stores the flag resulting from the [Curve Fit R2 outlier](#) condition evaluation. If [enabled by default](#) or by applying Outlier Setup, an associated column is highlighted.

## OutlierPeakNotFound

[OutlierPeakNotFound](#) stores the flag that indicates target peak is not found by integrator. If [enabled by default](#) or by applying Outlier Setup, an associated column is highlighted.

## OutlierRelativeResponseFactor

[OutlierRelativeResponseFactor](#) stores the flag resulting from this [Relative Response Factor outlier](#) condition evaluation. If [enabled by default](#) or by applying Outlier Setup, an associated column is highlighted.

## OutlierRelativeStandardError

[OutlierRelativeStandardError](#) stores the flag resulting from this [Relative Standard Error](#) condition evaluation. If [enabled by default](#) or by applying Outlier Setup, an associated column is highlighted.

## OutlierResponseCheckBelowLimit

[OutlierResponseCheckBelowLimit](#) stores the flag resulting from the [ResponseCheckMinimum](#) condition evaluation. If [enabled by default](#) or by applying Outlier Setup, an associated column is highlighted.

## OutlierResponseFactor

[OutlierResponseFactor](#) stores the flag resulting from the [Response Factor outlier](#) condition evaluation. If [enabled by default](#) or by applying Outlier Setup, an associated column is highlighted.

# OutlierSaturationRecovery

[OutlierSaturationRecovery](#) stores the flag resulting from the Saturation Recovery outlier condition evaluation. If [enabled by default](#) or by applying Outlier Setup, an associated column is highlighted.

## PeakFilterThreshold

[PeakFilterThreshold](#) represents the type of threshold filter that is applied to the chromatogram peaks that were detected by the integrator. The choice of PeakFilterThreshold determines the interpretation of PeakFilterThresholdValue. The following choices of PeakFilterThreshold are available:

PeakFilterThreshold	Filter condition
PeakAreaAbsThreshold	Peaks with area less than PeakFilterThresholdValue are filtered out
PeakAreaPctThreshold (default)	Peaks whose area, divided by maximum peak area, is less than PeakFilterThresholdValue/100 are filtered out
PeakHeightAbsThreshold	Peaks with height less than PeakFilterThresholdValue are filtered out
PeakHeightPctThreshold	Peaks whose height, divided by maximum peak height, is less than PeakFilterThresholdValue/100 are filtered out

Enum Name	UI Name	XPath expression
PeakAreaAbsThreshold	PeakAreaAbsThreshold	*//PeakFilterThreshold[.='PeakAreaAbsThreshold']
PeakAreaPctThreshold	PeakAreaPctThreshold	*//PeakFilterThreshold[.='PeakAreaPctThreshold']
PeakHeightAbsThreshold	PeakHeightAbsThreshold	*//PeakFilterThreshold[.='PeakHeightAbsThreshold']
PeakHeightPctThreshold	PeakHeightPctThreshold	*//PeakFilterThreshold[.='PeakHeightPctThreshold']

## PeakFilterThresholdValue

[PeakFilterThresholdValue](#) represents the threshold that is applied to the peak area or height, depending on the choice of PeakFilterThreshold. Chromatogram peaks that are below the PeakFilterThresholdValue are filtered out and are not considered as candidate peaks for quantitation.

## PeakSelectionCriterion

[PeakSelectionCriterion](#) represents the algorithm employed to select the peak which is designated the "hit" i.e. the [PrimaryHitPeakID](#). The criteria affect the mechanism of ranking the Peak rows associated with this TargetCompound row. The most suitable Peak row is then chosen as the primary "hit".

PeakSelectionCriterion has several possible values:

PeakSelectionCriterion	Value
GreatestResponse	GreatestResponse causes the ranking of the peaks such that the Peak row that exhibits the greatest integrator-determined response. For response, either height or area will be used as indicated by the value of the QuantitateByHeight column. This is the default value.  Note there is only one primary "hit". Other non-"hit" peaks are considered alternative "hits".
Close RT	Close RT causes the ranking of the peaks such that the Peak row that exhibits the closest integrator-determined retention time, irrespective of quality and fidelity of qualifier signal ratios is designated the "hit".  Note that other non-"hit" peaks are considered alternative "hits".
Close RT with Qualifiers	Close RT with Qualifiers causes the ranking of the peaks such that the Peak row that exhibits the best retention time among the Peak rows for which all qualifier ratio tolerances are satisfied is designated the "hit".  In the degenerate case in which there are no Peak row which are so Qualified, this ranking algorithm will be equivalent to Close RT.
Greatest Q-Value	Greatest Q-Value causes the ranking of the peaks such that the Peak row that exhibits the nominal qualifier

	<p>ratios that are best satisfied by the actual ratios. A correlation computation called QVALUE is performed to measure the fidelity of the observed qualifier ratios versus the nominal qualifier ratios.</p> <p>The definition of the QVALUE function is a well-defined statistic which yields a efficient measure of the "goodness of fit" of the observed qualifier ratios to the nominal qualifier ratios.</p>
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### Examples:

Changing the peak selection criterion from Greatest Response to Close RT for the target compound and for the ISTD helps avoid the larger spurious peaks.

Enum Name	UI Name	XPath expression
GreatestResponse	Greatest Response	*//PeakSelectionCriterion[.='GreatestResponse']
CloseRT	Close RT	*//PeakSelectionCriterion[.='CloseRT']
CloseRTQual	Close RT with Qualifiers	*//PeakSelectionCriterion[.='CloseRTQual']
GreatestQValue	Greatest Q-Value	*//PeakSelectionCriterion[.='GreatestQValue']

## PlatesCalculationType

[PlatesCalculationType](#) represents the choices of formulas used by different pharmacopeia to calculate the theoretical plates number. The following types are available:

Pharmacopeia	Formula
Default	$16 * (Tr / Wb) ^2$
USP	$16 * (Tr / Wb) ^2$
EU	$5.54 * (Tr / W50) ^2$
JP	$5.54 * (Tr / W50) ^2$

Tr is the retention time

Wb is the peak width determine by the tangent method.

W50 is the peak width at 50% of the height of the peak.

## PlatesLimit

[PlatesLimit](#) records the outlier limits for the Plates outlier.

## PrimaryHitPeakID

[PrimaryHitPeakID](#) is a link to a single Peak table row with which this TargetCompound row is associated. The Peak table row so identified is that Peak table row which is selected by the Quantitation process for quantitating the compound represented by this TargetCompound row.

If the value of PrimaryHitPeakID is `NULL`, there are either no hits or the quantitation has not yet been performed.

The assignment of the PrimaryHitPeakID is affected by the criteria set by the [PeakSelectionCriterion](#).

## PubChemID

[PubChemID](#) stores the PubChem identification.

## QCLCSMaximumRecoveryA

[QCLCSMaximumRecoveryA](#) represents the upper limit for the QC Laboratory Control Spike outlier. OutlierQCLCSRecoveryOutOfLimits is flagged if the recovery of a compound in a QC LCSA sample is higher than QCLCSMaximumRecoveryA.

## QCLCSMaximumRecoveryB

[QCLCSMaximumRecoveryB](#) represents the upper limit for the QC Laboratory Control Spike outlier. OutlierQCLCSRecoveryOutOfLimits is flagged if the recovery of a compound in a QC LCSB sample is higher than QCLCSMaximumRecoveryB.

## QCLCSMinimumRecoveryA

[QCLCSMinimumRecoveryA](#) represents the lower limit for the QC Laboratory Control Spike outlier. OutlierQCLCSRecoveryOutOfLimits is flagged if the recovery of a compound in a QC LCSA sample is lower than QCLCSMinimumRecoveryA.

## QCLCSMinimumRecoveryB

[QCLCSMinimumRecoveryB](#) represents the lower limit for the QC Laboratory Control Spike outlier. OutlierQCLCSRecoveryOutOfLimits is flagged if the recovery of a compound in a QC LCSB sample is lower than QCLCSMinimumRecoveryB.

## QCMaximumDeviation

[QCMaximumDeviation](#) represents the limit for the QC outlier. OutlierQCOutOfLimits is flagged if the CalculatedConcentration of a target compound in a QC sample differs from ExpectedConcentration by more than QCMaximumDeviation.

## QCMaximumPercentRSD

[QCMaximumPercentRSD](#) represents a setup parameter that affects the calculation of the QC Maximum Percent Relative Standard Deviation outlier. For details, please see the outlier description.

## QualifierRatioMethod

[QualifierRatioMethod](#) represents the algorithm chosen to evaluate ratios of qualifier signals to the target signal for this TargetCompound row. QualifierRatioMethod is an integer value representing one of four possible means of determining these qualifier ratios. A value of 0 for QualifierRatioMethod will determine the observed qualifier ratios by simple divisions of integrator-determined responses. Sets of ratios will be computed for each Peak row linked to this TargetCompound row. For each Peak row, a set of observed qualifier ratios will be determined by dividing, in turn, the response of each qualifier represented by a linked PeakQualifier row against the integrator-determined response of the Peak row itself. The response value will be height or area as indicated by the value of the QuantitateByHeight column. A value of 1, 2, or 3 for QualifierRatioMethod will compute the sets of observed qualifier ratios using Mass Spectrum peak ratios in lieu of the chromatographic-peak ratios used directly from the qualifier signals which are used in case (0). From the integration results, the retention times of the START, TOP, and END of the peak are retrieved. Spectra from the data source used in this quantitation experiment are extracted at each of those retention times. The intensities ("mass peaks") for the mass-to-charge domain value given by the MZ column are considered. For qualifier  $Q_i$ , let these intensities be  $start(Q_i)$ ,  $top(Q_i)$ , and  $end(Q_i)$ . For target, let these ratios be  $start(T)$ ,  $top(T)$ , and  $end(T)$ . A value of 1 computes each qualifier ratio as  $top(Q_i) /$



top(T). A value of 2 computes each qualifier ratio as  $(\text{top}(Q_i) - \text{LowFirstLast}(Q_i)) / (\text{top}(T) - \text{LowFirstLast}(T))$  where  $\text{LowFirstLast}(x) = \min(\text{start}(x), \text{end}(x))$  A value of 3 computes each qualifier ratio as  $(\text{top}(Q_i) - \text{AvgFirstLast}(Q_i)) / (\text{top}(T) - \text{AvgFirstLast}(T))$  where  $\text{AvgFirstLast}(x) = (\text{start}(x) + \text{end}(x)) / 2$

QualifierRatioMethod *feature is not currently supported.*

## QuantitateByHeight

[QuantitateByHeight](#) represents a flag indicating whether peak height or peak area is used as the response for purposes of quantitation. For a value of false, area is used for quantitation. For a value of true, height is used for quantitation. The choice of area or height applies to all TargetQualifier rows associated with this TargetCompound row.

## QuantitationMessage

[QuantitationMessage](#) represents a human-readable string that contains a list of the error messages (if any) that resulted from this compound's quantitation. If the compound was quantitated successfully, QuantitationMessage is NULL. If there are quantitation errors, QuantitationMessage contains a concatenation of all the error messages, one message per line, prefixed with the compound name. This string is subject to localization in other supported languages. Some examples of quantitation errors that may appear in the QuantitationMessage in English are summarized in the table below.

Quantitation Message	Explanation
Integrator did not find any peaks	The integrator could not find any peaks in the chromatogram extracted at this compound's target M/Z value (defined by the MZ column)
Qualifier M/Z=123: Integrator did not find any peaks	The integrator could not find any peaks in the chromatogram extracted at this qualifier's M/Z value
Qualifier M/Z=123: Qualifier peak not found or does not match quantitation criteria	The qualifier peak does not satisfy the qualifier selection criteria for successful compound quantitation, such as qualifier response ratio or retention time range.
Response is outside the range of the calibration curve fit	The response of the compound's primary peak cannot be converted to a concentration value on the calibration curve. This can occur for a quadratic curve fit, for example, if the target response is below the bottom or above the top of the parabola.

## QValueMinimum

[QValueMinimum](#) represents the lower limit for the Q Value outlier.

## ReferenceMSPathName

[ReferenceMSPathName](#) represents a persistent store containing a serialized or otherwise archived image of a Reference Mass Spectrum associated with the chemical compound indicated by this TargetCompound row.

*ReferenceMSPathName is not yet utilized in MS/MS product.*

## ReferenceWindowOverride

[ReferenceWindowOverride](#) is a compound level reference window setting, when it is not null, global nonReferenceWindow setting is overridden, and specified number is applied to this compound only.

## RelativeISTDMultiplier

[RelativeISTDMultiplier](#) affects only [RelativeISTD](#) analysis.

For Relative ISTD analysis, RelativeISTDMultiplier enters into the [CalculatedConcentration](#) determination.

$$\frac{\text{Response}}{\text{ISTDResponse}} * \text{ISTDConcentration} * \text{ISTDRelativeMultiplier} = \text{CalculatedConcentration}$$

Although the ISTD is often a heavy deuterated or carbon-13 analog, the ISTD can deliver a different response for the same amount of light or heavy compound. Hence, the RelativeISTDMultiplier offers a compound-based adjustment for Relative ISTD analysis.

## RelativeResponseFactorMaximumPercentDeviation

[RelativeResponseFactorMaximumPercentDeviation](#) serves as the limit for the Relative Response Factor outlier. RelativeResponseFactorMaximumPercentDeviation represents the maximum allowed deviation of the relative response factor for any calibration row of this compound from AverageRelativeResponseFactor.

# RelativeRetentionTimeMaximumPercentDeviation

[RelativeRetentionTimeMaximumPercentDeviation](#) serves as the limit for the Relative Retention Time outlier. RelativeRetentionTimeMaximumPercentDeviation represents the maximum allowed relative percent deviation of the relative retention time of this compound from AverageRelativeRetentionTime.

# RelativeStandardError

[RelativeStandardError](#) represents a metric for the calibration curve fitting. The calculation is as follows:

$$\%RSE = 100 \times \sqrt{\sum_{i=1}^n \left[ \frac{x'_i - x_i}{x_i} \right]^2 / (n - p)}$$

$x_i$  = True value of the calibration level  $i$

$x'_i$  = Measured concentration of calibration level  $i$

$p$  = Number of terms in the fitting equation  
(average = 1, linear = 2, quadratic = 3)

$n$  = Number of calibration points

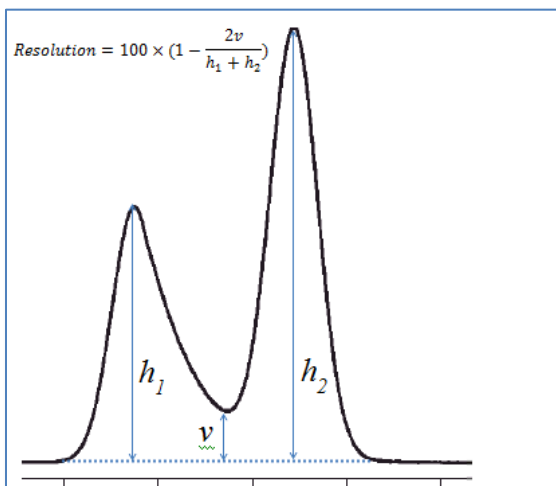
# RelativeStandardErrorMaximum

[RelativeStandardErrorMaximum](#) represents an outlier upper limit for the RSE% outlier.

# ResolutionCalculationType

[ResolutionCalculationType](#) represents the choices of formulas used by different pharmacopedia to calculate the peak resolution. The following types are available:

Default:



$$USP: 2 * (Tr,2 - Tr,1) / (Wb,1 + Wb,2)$$

JP:  $1.18 * (Tr, 2 - Tr, 1) / (W50,1 + W50,2)$

EU:  $1.18 * (Tr, 2 - Tr, 1) / (W50,1 + W50,2)$

Valley Height/Peak Height:  $v / \text{height of target peak}$

Valley Height/Peak Height Average:  $100 * 2 * \frac{v}{h_1+h_2}$

Valley Height/Peak Height Sum:  $100 * \frac{v}{h_1+h_2}$

## ResolutionLimit

[ResolutionLimit](#) serves as the limit for the Peak Resolution Below Limit outlier.

## ResponseCheckMinimum

[ResponseCheckMinimum](#) serves as the limit for the Response Check Below Limit outlier.

## ResponseFactorMaximumPercentDeviation

[ResponseFactorMaximumPercentDeviation](#) serves as the limit for the Response Factor outlier. ResponseFactorMaximumPercentDeviation represents the maximum allowed deviation of the response factor for any calibration row of this compound from AverageResponseFactor.

## ResponseFactorRSD

[ResponseFactorRSD](#) represents the relative standard deviation of Response Factor for enabled calibration levels.

## RetentionIndex

[RetentionIndex](#) records the back-calculated retention index as determined from the library search.

LibraryRetentionIndex requires the compound is perceived using a retention time calibration (RT CAL).

## RetentionTime

[RetentionTime](#) represents, in units of minutes, the chromatographic retention time at which the chromatographic peak for this TargetCompound row is associated. Note that for a TargetCompound row for which ISTDCompoundID is not `NULL`, this nominal retention time is subject to modulation by the ratio of the observed and nominal retention times of the related Internal Standard compound. This ratio is readily available by querying the retention-time information stored in the so-indicated internal-standard TargetCompound row and its associated primary-hit Peak row. Default value is 0.

## RetentionTimeDeltaUnits

[RetentionTimeDeltaUnits](#) represents the choice of units for LeftRetentionTimeDelta and RightRetentionTimeDelta. The choices are Minutes or Percent. If RetentionTimeDeltaUnits is set to Minutes, the values of LeftRetentionTimeDelta and RightRetentionTimeDelta are interpreted as an offset in minutes from RetentionTime. If RetentionTimeDeltaUnits is set to Percent, the values of LeftRetentionTimeDelta and RightRetentionTimeDelta are interpreted as a percentage offset from RetentionTime.

Enum Name	UI Name	XPath expression
Minutes	Minutes	*//RetentionTimeDeltaUnits[.='Minutes']
Percent	Percent	*//RetentionTimeDeltaUnits[.='Percent']

## RetentionTimeWindow

[RetentionTimeWindow](#) represents the full width of the range of allowed values of RetentionTime. RetentionTimeWindow serves to define the limits for the Retention Time outlier condition.

## RetentionTimeWindowCC

[RetentionTimeWindowCC](#) represents the full width of the range of allowed values of RetentionTime for CC SampleType. RetentionTimeWindowCC serves to define the limits for the Retention Time CC outlier condition.

## RetentionTimeWindowUnits

[RetentionTimeWindowUnits](#) represents the choice of units for RetentionTimeWindow. The choices are Minutes or Percent. If RetentionTimeWindowUnits is set to Minutes, the value of RetentionTimeWindow is interpreted as an offset in minutes from RetentionTime. If RetentionTimeWindowUnits is set to Percent, the value of RetentionTimeWindow is interpreted as a percentage offset from RetentionTime.

Enum Name	UI Name	XPath expression
Percent	Percent	*//RetentionTimeWindowUnits[.='Percent']
Minutes	Minutes	*//RetentionTimeWindowUnits[.='Minutes']



## RightRetentionTimeDelta

[RightRetentionTimeDelta](#) represents time expressed in units of minutes or percent of nominal RetentionTime, as indicated by RetentionTimeDeltaUnits. It defines the offset used to determine the upper bound for the retention-time window for signals which are extracted in support of quantitating the chemical compound indicated by this TargetCompound row.

### Example:

RetentionTime has a value of 5 minutes. RightRetentionTimeDelta has a value of 0.1 and RetentionTimeDeltaUnits has a value of 0 for Minutes. Then the upper bound on the extraction window is  $5 + 0.1$  or 5.1 minutes. On the other hand if RetentionTimeDeltaUnits is 1 for Percent and RightRetentionTimeDelta is 20, then the upper bound on the extraction window is  $5 + 20\% * 5 = 6$  minutes. Default value is 1 minutes.

## RxUnlabeledIsotopicDilution

[RxUnlabeledIsotopicDilution](#) is the Rx value used in calculations for Stable Labeled Isotope quantitation technique. A full [discussion](#) of that technique is beyond the scope of this document.

## RyLabeledIsotopicDilution

[RyLabeledIsotopicDilution](#) is the RY value used in calculations for Stable Labeled Isotope quantitation technique. A full [discussion](#) of that technique is beyond the scope of this document.

## SampleAmountLimitHigh

[SampleAmountLimitHigh](#) represents the upper limit for the Sample Amount outlier.

OutlierSampleAmountOutOfLimits is set to High if the FinalConcentration of this compound exceeds SampleAmountLimitHigh.

## SampleAmountLimitLow

[SampleAmountLimitLow](#) represents the lower limit for the Sample Amount outlier.

OutlierSampleAmountOutOfLimits is set to Low if the FinalConcentration of this compound is less than SampleAmountLimitLow.

## SampleMaximumPercentRSD

[SampleMaximumPercentRSD](#) represents the upper limit for the SampleRSD outlier.

[OutlierSampleOutsideRSD](#) is set to High if the [SampleRSD](#) of this compound in the batch is higher than SampleMaximumPercentRSD.

## ScanType

[ScanType](#) represents a human-readable string describing the experimental technique used to collect the data used to analyze the chemical compound represented by this TargetCompound row. Possible values include "MRM", "SRM", "Parent Ion Scan", or "Neutral Loss Scan". This string is subject to localization in other supported languages.

Enum Name	UI Name	XPath expression
MRM	MRM	*//ScanType[.='MRM']
NeutralLoss	Neutral Loss	*//ScanType[.='NeutralLoss']
NeutralGain	Neutral Gain	*//ScanType[.='NeutralGain']
ProductIon	Product Ion	*//ScanType[.='ProductIon']
PrecursorIon	Precursor Ion	*//ScanType[.='PrecursorIon']
Ms1Scan	Ms1 Scan	*//ScanType[.='Ms1Scan']
Ms2Scan	Ms2 Scan	*//ScanType[.='Ms2Scan']
Ms1SIM	Ms1 SIM	*//ScanType[.='Ms1SIM']
Ms2SIM	Ms2 SIM	*//ScanType[.='Ms2SIM']

## SelectedMZ

[SelectedMZ](#) represents a mass-to-charge measurement, in units of daltons per unit charge, of the ions selected by the first-quadrupole stage in a tandem mass spectrometer used to perform this experiment.

## SignalInstance

[SignalInstance](#) identifies which of several detectors of the same type to use. SignalInstance is useful when there are two (or more) signals from the same kind of detector. For example, two Flame Ionization Detectors (FID).

SignalInstance is `NULL` by default. If SignalInstance is `NULL`, the instance is set to 1 by default.

{[SignalType](#), [SignalName](#), [SignalInstance](#)} together uniquely identify the signal.

# SignalName

[SignalName](#) represents a particular part of the signal as defined by [SignalType](#). For example, for the variable wavelength detectors for liquid chromatography (LC), the different wavelengths are labeled "A", "B", "C"... Hence, SignalName specifies the actual wavelength within the entire Variable Wavelength Detector (VWD) [SignalType](#).

SignalName is `NULL` by default. If SignalName is `NULL`, the first signal name for the currently defined signal type is used. For MS [SignalType](#), SignalName is ignored.

# SignalRetentionTimeOffset

[SignalRetentionTimeOffset](#) is for future feature.

# SignalToNoiseMultiplier

[SignalToNoiseMultiplier](#) is a multiplier for signal to noise ratio. If a value is set in the "S/N Multiplier", the final signal-to-noise value will be multiplied by the set value. For example, to calculate the signal-to-noise as  $S/N = 2H/h$  with:

- H is the peak height.
- h is the noise value.

Set the "S/N Multiplier" value to "2.0".

# SignalType

[SignalType](#) represents a type of signal acquired from a particular detector.. By default, the signal is MS. Additional signal types include two dimensional (2D) signals such as Flame Ionization Detector (FID). Further delineation of the SignalType is identified using the [SignalName](#).

Below is a list of acronyms for SignalTypes. Note that the list does not imply support.

ADC = Analogy to Digital Converter

DAD = Diode Array Detector

ECD = Electron Capture Detector

FID = Flame Ionization Detector

FLD = Fluorescence Detector

FPD = Flame Photometric Detector

MWD = Multiple Wavelength Detector

**MS = Mass Spectrometer Detector (default)**

NPD = Nitrogen Phosphorus Detector

RID = Refractive Index Detector

PID = Photo Ionization Detector

TCD = Thermal Conductivity Detector

VWD = Variable Wavelength Detector

UNK = Unknown



# Smoothing

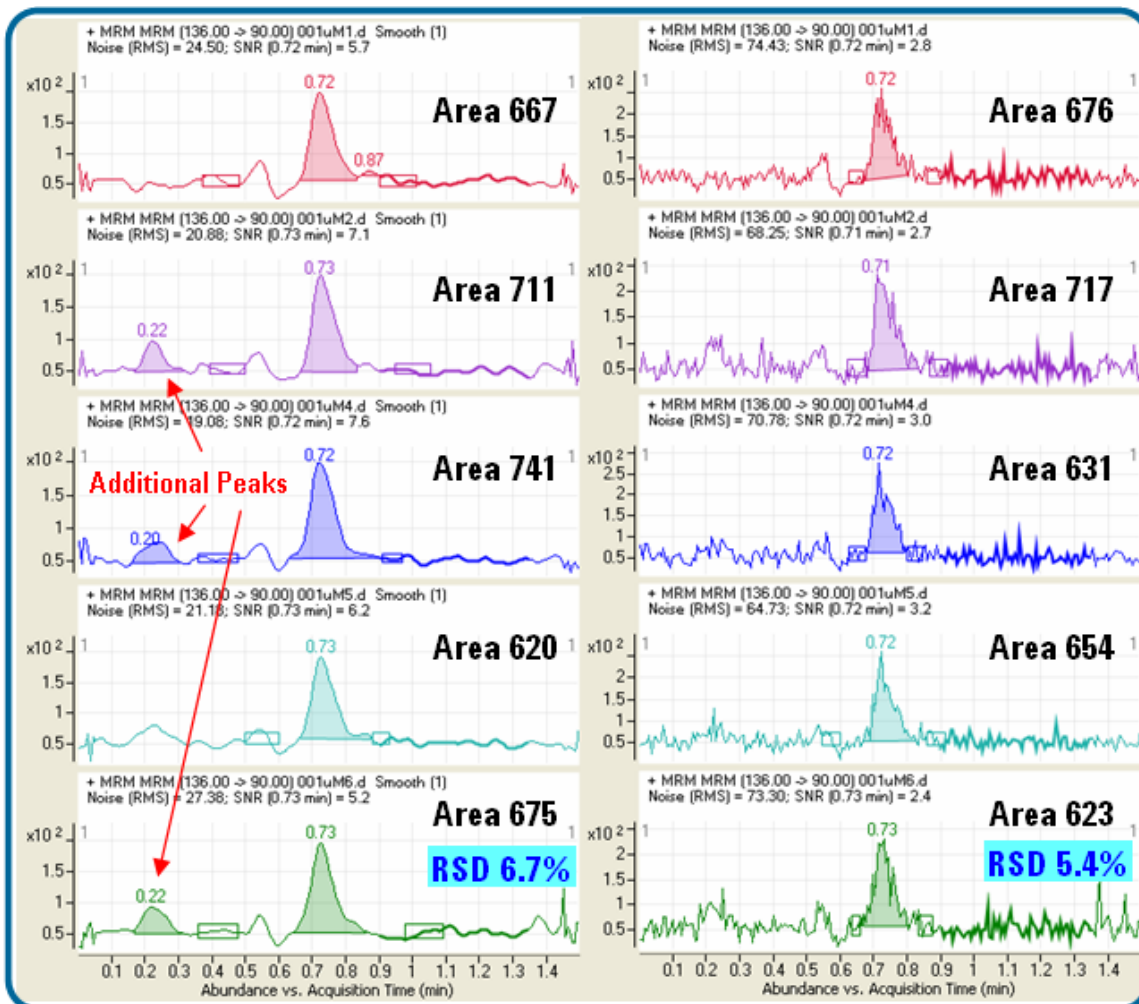
[Smoothing](#) represents the smoothing algorithm applied.

Choices include:

- None (default)
- Gaussian
- Quadratic/Cubic Savitzsky-Golay
- Quartic/Quintic Savitzsky-Golay

Qualifier chromatograms are smoothed using the same parameters as the target compound.

**Warning:** Smoothing is not recommended with the parameter-less integrator.



**Smooth:** Comparison of parameter-less integrator with and without previous smoothing on 5 injection of 670 fg of Homocysteine (transition 136 > 90 m/z) on column.

Smoothing is not recommended since it will reduce the frequency domain of noise and spikes and may results in additional integrated peaks. As can be seen, the RSDs for repetitive injections are similar or even smaller when integrating unsmoothed chromatograms compared to smoothed data.

Enum Name	UI Name	XPath expression
None	'None'	*//@Smoothing[.='None']
Gaussian	Gaussian	*//@Smoothing[.='Gaussian']
SavitzkyGolay23	Quadratic/Cubic Savitzsky-Golay	*//@Smoothing[.='SavitzkyGolay23']
SavitzkyGolay45	Quartic/Quintic Savitzsky-Golay	*//@Smoothing[.='SavitzkyGolay45']

## SmoothingFunctionWidth

[SmoothingFunctionWidth](#) represents the width of the moving weighted averaged window.

The function width defines how many points are averaged at each smoothing step. So if the function width is 5, then:

- a.) The first five points (0, 1, ..., 4) are averaged (with appropriate weights). The result is the value in the output object for the middle point of that group (the point with index = 2).
- b.) The next group of five points (1, 2, ..., 5) are averaged to get the new value for point 3
- c.) The next group of five points (2, 3, ..., 6) are averaged ...

SmoothingFunctionWidth must be at least 4 for SavitzskyGolay23 and at least 6 for SavitzskyGolay45 (enforced by method validation)

## SmoothingGaussianWidth

[SmoothingGaussianWidth](#) represents the width of the Gaussian function.

[SmoothingGaussianWidth](#) weights are calculated to give a smoothing function that is Gaussian in shape, with a specified width. The width is specified as the "Gaussian width", and is in units of "points". I.e., a value of 3.5 specifies a Gaussian whose width is 3.5 times the spacing of the points.

[SmoothingGaussianWidth](#) must be positive and not greater than SmoothingFunctionWidth.



## Species

[Species](#) represents the adduct type of the target compound.

## SpectrumBaselineThreshold

[SpectrumBaselineThreshold](#) represents the counts to be subtracted in a point-to-point manner before spectrum extraction. In Quantitation software, this parameter defaults to null.

## SpectrumExtractionOverride

[SpectrumExtractionOverride](#) represents what spectrum is used to calculate the reference library match score and in conjunction with the "Override spectrum" checkbox in the Compound Information Properties dialog box, it determines which spectrum is displayed in the Compound Information Window.

If the field is left empty or set to "Default" the Spectrum Extraction Override has no effect and the spectrum extracted to calculate the Library Match Score is based on the Scan Type defined in the method.

If the field is set to "Scan", the "Scan" spectrum is extracted (if present in the data file) to calculate the Library Match Score, overriding the Scan Type defined in the method. For example, processing SIM/Scan data.

If the field is set to "Product Ion", the "Product Ion" spectrum is extracted (if present in the data file) to calculate the Library Match Score, overriding the Scan Type defined in the method. For example, processing Targeted MS/MS data.

If the field is set to "Deconvoluted Scan", deconvolution will be run and a component spectrum (if found) will be used to calculate the Library Match Score.

Note that this field has no effect if a valid Reference Library is not set in the Globals Setup.

## SpectrumScanInclusion

[SpectrumScanInclusion](#) represents how spectrum is extracted. [SpectrumScanInclusion](#) defaults to "Average", where spectrum is average of all spectra within defined RT range. If [SpectrumScanInclusion](#) is set to "Apex", it extracts a single spectrum from the top of the peak.

## SpectrumPeakHeightPercentThreshold

[SpectrumPeakHeightPercentThreshold](#) represents the percentage of the peak height to use to extract and average spectra. When this parameter is set, the average spectrum will include spectra within the RT range where all points on the EIC is above the specified percentage of peak height. In TOF/QTOF flavors, it defaults to 10%.

## SpectrumPercentSaturationThreshold

[SpectrumPercentSaturationThreshold](#) represents the maximum percentage of saturation to include in the average. If a peak in the spectrum is above the given percentage of being saturated, that spectrum will be excluded from the average.

If a Reference Pattern Library is specified in the method, only masses (+/- MZExtractionWindow) in the pattern library are monitored for saturation. For other masses even though their abundances could be above saturation limit, the scan lines are not excluded from average since they are not contributing to the accurate mass match scores.

If mass accuracy outlier or reference library is specified, only target ion and qualifier ions (+/- MZExtractionWindow) are monitored for saturation when calculating average spectrum.

In TOF/QTOF flavors, it defaults to 10%.

## SpectrumQuantifierQualifierOnly

[SpectrumQuantifierQualifierOnly](#) is a Boolean flag. If it is true, compound spectrum is filtered to include quantifier and qualifiers only for the library match score.

## SubList

[SubList](#) is a Boolean flag that can categorize compounds as part of a particular set of the compounds in the quantitation method.

The column does not have any effect on any calculation, but potentially can be used for report customization.

For example, mark a set of compounds to designate they are on/off a list.

Note that the Sublist column displays as "OnOff" in UI.

## SurrogateConcentration

[SurrogateConcentration](#) represents the expected concentration of this surrogate compound, expressed in units of ConcentrationUnits. SurrogateConcentration is used to evaluate the Surrogate outlier and Surrogate Percent Recovery outlier conditions. SurrogateConcentration is only meaningful for compounds of type Surrogate.

## SurrogateConcentrationLimitHigh

[SurrogateConcentrationLimitHigh](#) represents the upper limit for the Surrogate outlier.

[OutlierSurrogateOutOfLimits](#) is set to High if the [FinalConcentration](#) of this compound exceeds SurrogateConcentrationLimitHigh.

## SurrogateConcentrationLimitLow

[SurrogateConcentrationLimitLow](#) represents the lower limit for the Surrogate outlier.

[OutlierSurrogateOutOfLimits](#) is set to Low if the FinalConcentration of this compound is less than SurrogateConcentrationLimitLow.

## SurrogatePercentRecoveryMaximum

[SurrogatePercentRecoveryMaximum](#) represents the upper limit for the Surrogate Percent Recovery outlier. [OutlierSurrogatePercentRecovery](#) is set to High if the FinalConcentration of this compound exceeds SurrogatePercentRecoveryMaximum.

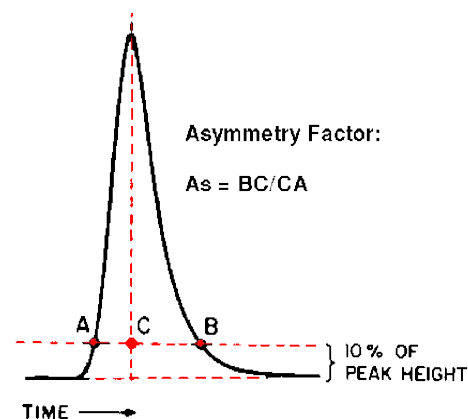
## SurrogatePercentRecoveryMinimum

[SurrogatePercentRecoveryMinimum](#) represents the lower limit for the Surrogate Percent Recovery outlier. [OutlierSurrogatePercentRecovery](#) is set to Low if the FinalConcentration of this compound is less than SurrogatePercentRecoveryMinimum.

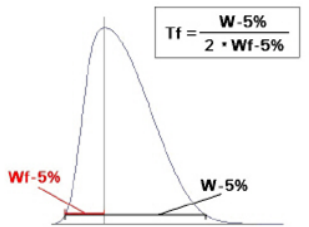
## SymmetryCalculationType

[SymmetryCalculationType](#) represents the choices of formulas used by different pharmacopedia to calculate the peak symmetry (tailing factor). The following types are available:

Default:



USP/JP/EU:



- W-5 is the peak width at 5% height of the peak.
- Wf-5% is the front peak width at 5% height of the peak.

## SymmetryLimitHigh

[SymmetryLimitHigh](#) represents the higher limit which indicates tailing for the Symmetry outlier. [OutlierSymmetry](#) is set to High if the calculated [Symmetry](#) value of the primary peak is greater than the SymmetryLimitHigh.

## SymmetryLimitLow

[SymmetryLimitLow](#) represents the lower limit which indicates fronting for the Symmetry outlier. [OutlierSymmetry](#) is set to Low if the calculated [Symmetry](#) value of the primary peak is less than the SymmetryLimitLow.

## TargetCompoundIDStatus

[TargetCompoundIDStatus](#) is an internal string.

## ThresholdNumberOfPeaks

[ThresholdNumberOfPeaks](#) represents a Peak Filter parameter that defines the maximum number of chromatogram peaks retained by the integrator.

### Example:

If ThresholdNumberOfPeaks is set to 10, then of all the peaks that are found by the integrator, up to a maximum of 10 largest peaks shall be passed to the Quantitation Engine.

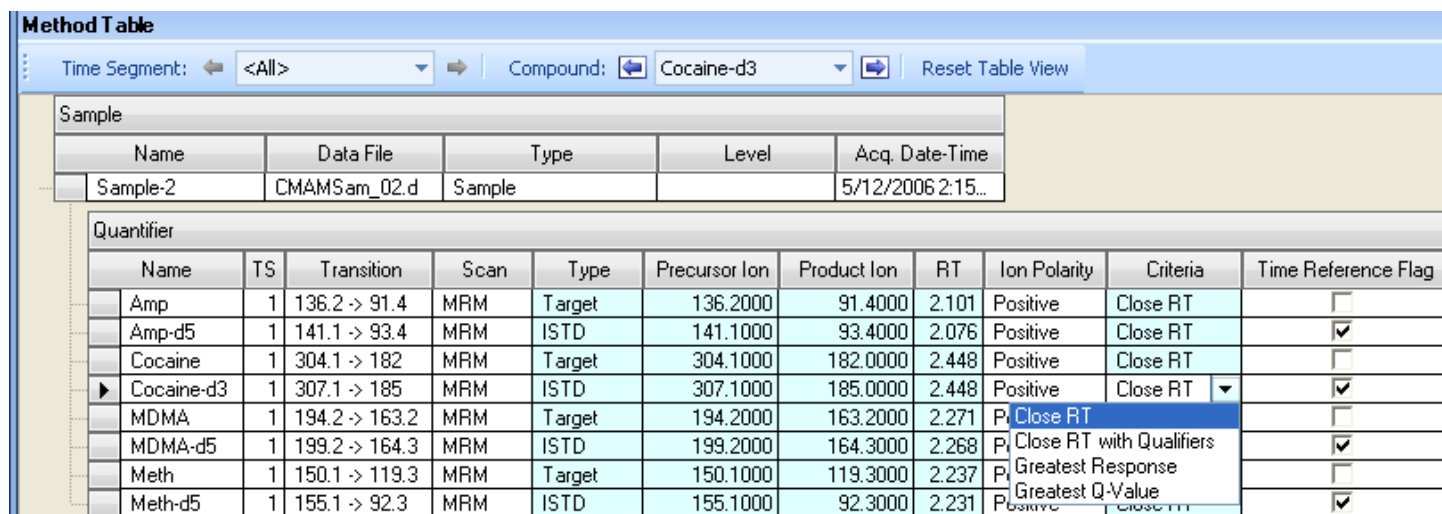
# TimeReferenceFlag

[TimeReferenceFlag](#) has the value true if and only if this TargetCompound row represents a time reference compound. Only internal standard compounds can be designated as time reference compounds.

If compound B is a time reference for compound A, then the Quantitation Engine will multiply the retention time of A's peaks by the ratio of the actual-to-expected retention time of B's primary hit peak.

TimeReference allows a time correction for a particular target compound. The approach is useful in the case where the target compound's retention time drifts and the related ISTD used as the time reference also experiences the same relative shift. As a result, the Quantitation Engine will look for this target compound in a shifted retention time.

Note that the extract retention time window does not shift, just the retention time where the target is expected. With the Peak Selection criteria set to Closest Retention Time, this shift in the expected retention time can improve the peak selection, especially when another peak exists in the same extracted chromatogram.



The screenshot shows the 'Method Table' interface with the following controls and data:

Time Segment: <All>    Compound: Cocaine-d3    Reset Table View

Sample				
Name	Data File	Type	Level	Acq. Date-Time
Sample-2	CMAMSam_02.d	Sample		5/12/2006 2:15...

Quantifier										
Name	TS	Transition	Scan	Type	Precursor Ion	Product Ion	RT	Ion Polarity	Criteria	Time Reference Flag
Amp	1	136.2 -> 91.4	MRM	Target	136.2000	91.4000	2.101	Positive	Close RT	<input type="checkbox"/>
Amp-d5	1	141.1 -> 93.4	MRM	ISTD	141.1000	93.4000	2.076	Positive	Close RT	<input checked="" type="checkbox"/>
Cocaine	1	304.1 -> 182	MRM	Target	304.1000	182.0000	2.448	Positive	Close RT	<input type="checkbox"/>
Cocaine-d3	1	307.1 -> 185	MRM	ISTD	307.1000	185.0000	2.448	Positive	Close RT	<input checked="" type="checkbox"/>
MDMA	1	194.2 -> 163.2	MRM	Target	194.2000	163.2000	2.271	Positive	Close RT	<input type="checkbox"/>
MDMA-d5	1	199.2 -> 164.3	MRM	ISTD	199.2000	164.3000	2.268	Positive	Close RT with Qualifiers	<input checked="" type="checkbox"/>
Meth	1	150.1 -> 119.3	MRM	Target	150.1000	119.3000	2.237	Positive	Greatest Response	<input type="checkbox"/>
Meth-d5	1	155.1 -> 92.3	MRM	ISTD	155.1000	92.3000	2.231	Positive	Greatest Q-Value	<input checked="" type="checkbox"/>

**TimeReference: Application of Closest RT with ISTD TimeReference.**

# TimeSegment

[TimeSegment](#) represents the index of the acquisition time segment that was used to acquire the signal for this compound.

## Transition

[Transition](#) represents a human-readable string that expresses the M/Z values measured for this compound. The format of the Transition string depends on ScanType. When ScanType = MRM, the transition string has the format "SelectedMZ -> MZ", where SelectedMZ is the precursor ion and MZ is the product ion.

## TriggeredTransitions

[TriggeredTransitions is a comma-separated string](#) that represents Triggered MRM transitions. This column is populated automatically from the acquisition method when creating a new quantitation method from acquired MRM data. Values can also be entered manually.

When extracting a spectrum, if the TriggeredTransitions string is not null, it will be parsed and an EIC will be extracted for each triggered transition in the list. The latest start-of-data point in RT defines the trigger point, RT\_trigger, and the compound spectrum will be extracted over the RT range = [RT\_trigger, RT\_end], where RT\_end is the end of the primary target peak. For the (non-triggered) MRM case, the TriggeredTransitions column will be null and the spectrum extraction will occur as it normally does.

## UncertaintyRelativeOrAbsolute

[UncertaintyRelativeOrAbsolute](#) clarifies the specification of tolerance for actual vs. nominal qualifier signal ratios. Its value is Relative (default) or Absolute. This value applies to all TargetQualifier rows associated with this TargetCompound row.

### Example:

Consider a nominal qualifier signal ratio of 80 percent between Qualifier Q1 and this target compound, with a 20 per cent uncertainty. If UncertaintyRelativeOrAbsolute is Relative, then the tolerance bounds for the qualifier ratio are 64 to 96, because 20 per cent of 80 is 16. If UncertaintyRelativeOrAbsolute is Absolute, then the tolerance bounds for the qualifier ratio are 60 to 100, because 20 per cent uncertainty is treated as an absolute offset from 80 per cent.

Enum Name	UI Name	XPath expression
Absolute	Absolute	*//@UncertaintyRelativeOrAbsolute[.='Absolute']

Relative	Relative	*//@UncertaintyRelativeOrAbsolute[.='Relative']
----------	----------	---

## UserAnnotation

[UserAnnotation](#) stores an arbitrary user-defined string.

UserAnnotation is editable in Batch-at-a-Glance. It's a per compound per sample information.

If a method that contains User Annotation values is saved, the User Annotation values are removed when the method is opened and applied to a new batch.

## UserCustomCalculation

[UserCustomCalculation](#) stores a result from a custom calculation.

UserCustomCalculation work with a scripting mechanism requiring .NET Framework programming skills.

## UserCustomCalculationLimitHigh

[UserCustomCalculationLimitHigh](#) represents the upper limit for the triggered user custom calculation. Calculation producing results higher than the limit set the outlier to "High".

## UserCustomCalculationLimitLow

[UserCustomCalculationLimitLow](#) represents the upper limit for the triggered user custom calculation. Calculation producing results higher than the limit set the outlier to "Low".

## UserDefined

[UserDefined](#) stores an arbitrary user-defined string.

UserDefined is editable in Batch-at-a-Glance, on a per compound basis. If a method that contains User Defined values is saved, the User Defined values are retained when the method is opened and applied to a batch.

## UserDefined1

[UserDefined1](#) stores an arbitrary user-defined string.

UserDefined is editable in Batch-at-a-Glance, on a per compound basis. If a method that contains User Defined values is saved, the User Defined values are retained when the method is opened and applied to a batch.

## UserDefined2

[UserDefined2](#) stores an arbitrary user-defined string.

UserDefined is editable in Batch-at-a-Glance, on a per compound basis. If a method that contains User Defined values is saved, the User Defined values are retained when the method is opened and applied to a batch.



## UserDefined3

[UserDefined3](#) stores an arbitrary user-defined string.

UserDefined is editable in Batch-at-a-Glance, on a per compound basis. If a method that contains User Defined values is saved, the User Defined values are retained when the method is opened and applied to a batch.

## UserDefined4

[UserDefined4](#) stores an arbitrary user-defined string.

UserDefined is editable in Batch-at-a-Glance, on a per compound basis. If a method that contains User Defined values is saved, the User Defined values are retained when the method is opened and applied to a batch.

## UserDefined5

[UserDefined5](#) stores an arbitrary user-defined string.

UserDefined is editable in Batch-at-a-Glance, on a per compound basis. If a method that contains User Defined values is saved, the User Defined values are retained when the method is opened and applied to a batch.

## UserDefined6

[UserDefined6](#) stores an arbitrary user-defined string.

UserDefined is editable in Batch-at-a-Glance, on a per compound basis. If a method that contains User Defined values is saved, the User Defined values are retained when the method is opened and applied to a batch.

## UserDefined7

[UserDefined7](#) stores an arbitrary user-defined string.

UserDefined is editable in Batch-at-a-Glance, on a per compound basis. If a method that contains User Defined values is saved, the User Defined values are retained when the method is opened and applied to a batch.

## UserDefined8

[UserDefined8](#) stores an arbitrary user-defined string.

UserDefined is editable in Batch-at-a-Glance, on a per compound basis. If a method that contains User Defined values is saved, the User Defined values are retained when the method is opened and applied to a batch.

## UserDefined9

[UserDefined9](#) stores an arbitrary user-defined string.

UserDefined is editable in Batch-at-a-Glance, on a per compound basis. If a method that contains User Defined values is saved, the User Defined values are retained when the method is opened and applied to a batch.

## UserDefinedTargetCompoundID

[UserDefinedTargetCompoundID](#) stores a back pointer from dynamic target to the user-defined parent compound. Null for user-defined target compounds. For dynamic target compounds, points to the CompoundID of the "parent" (user-defined) target compound. Set at Method Setup time.

## VerifiedIonType

[VerifiedIonType](#) represents the different screening criteria type for the Number Of Verified Ions outlier. It's an Enum, and the two values are SANTE\_UnitMass and SANTE\_AccurateMass.

## WavelengthExtractionRangeHigh

[WavelengthExtractionRangeHigh](#) represents the wavelength that defines the high limit of the range used to extract the UV-vis spectral signal.

## WavelengthExtractionRangeLow

[WavelengthExtractionRangeLow](#) represents the wavelength that defines the low limit of the range used to extract the UV-vis spectral signal.

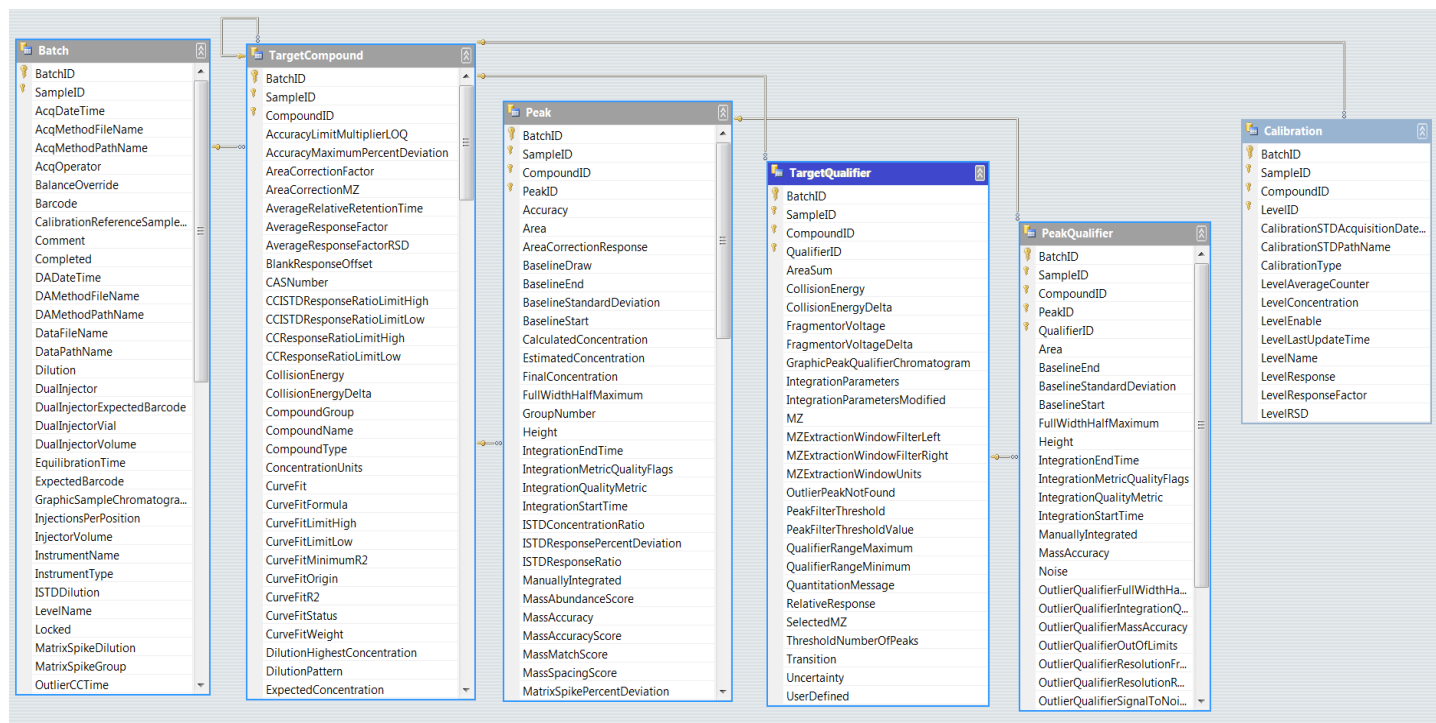
## WavelengthReferenceRangeHigh

[WavelengthReferenceRangeHigh](#) represents the wavelength that defines the high limit of the range used for the UV-vis spectral reference signal.

## WavelengthReferenceRangeLow

[WavelengthReferenceRangeLow](#) represents the wavelength that defines the low limit of the range used for the UV-vis spectral reference signal.

# TargetQualifier Table



## Primary Key

{[BatchID](#), [SampleID](#), [CompoundID](#), [QualifierID](#)} serves as the primary key. The composite of the [BatchID](#) and [SampleID](#) and [CompoundID](#) uniquely identify each row in this table. The keys in the Quantitation DataSet are not shown in the user interface.

A primary key value must be unique within the table. A composite key is a primary key that incorporates more than one column.

## BatchID

[BatchID](#) uniquely identifies the batch. [BatchID](#) is part of the composite primary key. The [BatchID](#) is typically set to -1 because Batch-at-a-Glance analyzes one batch.

## SampleID

[SampleID](#) uniquely identifies the sample in the batch. [SampleID](#) is part of the composite primary key. Thus, each sample in the batch is assigned a unique [SampleID](#).

## CompoundID

[CompoundID](#) uniquely identifies the sample in the batch. CompoundID is part of the composite primary key.

Thus, each compound in the batch is assigned a unique CompoundID.

## QualifierID

[QualifierID](#) uniquely identifies the qualifier(s) for this compound. QualifierID is part of the composite primary key. Thus, each qualifier for this compound is assigned a unique QualifierID.

## AreaSum

[AreaSum](#) controls summing of the qualifier response to the target response. AreaSum is false by default.

If this flag has a value of true, then for purposes of quantitation the qualifier response is accumulated with the response of the associated target signal (and possibly with responses of other qualifier signals also associated with the same target).

Note that the target peak displays as the target response, not the target plus qualifier summed responses. In addition, the qualifier ratio is also calculated in the same manner in either case, i.e. non-area summed or area summed, non summed area is always used for calculation of qualifier ratios.

## CellAcceleratorVoltage

[CellAcceleratorVoltage](#) represents a meta data from LCQQQ acquisition.

## CollisionEnergy

[CollisionEnergy](#) represents the amount of collision-induced dissociation (CID) occurring in the triple (QQQ) collision cell. CID is a mechanism to fragment molecular ions in the gas phase. The molecular ions are accelerated by this electrical potential to high kinetic energy in the vacuum of a mass spectrometer and to collide in the higher pressure collision cell with neutral gas molecules (nitrogen). In the collision some of the kinetic energy is converted into internal energy which results in bond breakage and the fragmentation of the molecular ion into smaller fragments.

## CollisionEnergyDelta

[CollisionEnergyDelta](#) defines the one-sided extend of the chromatograms/spectra extraction range of the CollisionEnergy. If this value is set, the actual extraction range of chromatograms and spectra is given by the following formula:

CE range = [CollisionEnergy – CollisionEnergyDelta, CollisionEnergy + CollisionEnergyDelta]

The quantifier and each of the qualifier ions can be assigned independent CE extraction ranges.

## FragmentorVoltage

[FragmentorVoltage](#) represents the acquisition parameter that controls the acceleration of the ions from the source into the rest of the mass spectrometer (mass analyzer and detection).

## FragmentorVoltageDelta

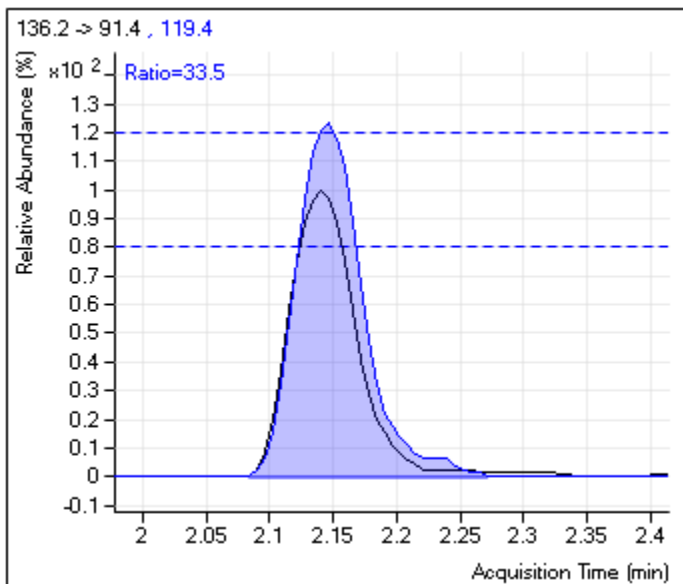
[FragmentorVoltageDelta](#) defines the one-sided extent of the chromatograms/spectra extraction range of the FragmentorVoltage. If this value is set, the actual extraction range of chromatograms and spectra is given by the following formula:

$$\text{FV range} = [\text{FragmentorVoltage} - \text{FragmentorVoltageDelta}, \text{FragmentorVoltage} + \text{FragmentorVoltageDelta}]$$

In this formula, the bottom of the FV range is constrained to be non-negative. The quantifier and each of the qualifier ions can be assigned independent FV extraction ranges.

## GraphicPeakQualifierChromatogram

[GraphicPeakQualifierChromatogram](#) represents a relative path and filename to a graphic (.emf) file used in reporting.



Graphic 6: File reference to graphic.

## IntegrationParameters

[IntegrationParameters](#) names a persistent store containing a collection of parameters to modulate the behavior of the integration algorithm brought to bear on the signal indicated by this TargetQualifier row. The default value for IntegrationParameters is `NULL`. Wherever this column is null, signal integration proceeds assuming the same integration settings as target quantifier ion are used.

## IntegrationParametersModified

[IntegrationParametersModified](#) is true when the integration parameters for a compound is modified at the sample level.

## IonPolarity

[IonPolarity](#) represents an acquisition parameter that records the polarity of the ions focused with voltages applied to a lens system located between the source and the analyzer. If null, IonPolarity of parent quantifier is used.

Enum Name	UI Name	XPath expression	Summary
Positive	Positive	*//IonPolarity[.='Positive']	Positive ion polarity
Negative	Negative	*//IonPolarity[.='Negative']	Negative ion polarity
Unassigned	Unassigned	*//IonPolarity[.='Unassigned']	Unknown ion polarity
Mixed	Mixed	*//IonPolarity[.='Mixed']	Contains both positive and negative ion polarity data

## MZ

[MZ](#) represents a mass-to-charge measurement in units of Daltons per unit charge, of the ions selected in the stage before the ions hit the detector.

In MRM, the combination of SelectMZ (precursor ion) and MZ (product ion) determine the transition.

For single quadrupole modes, MZ sets the mass filter for the ions.

MZ is analogous to and serves exactly the same role for the qualifier signal represented by this TargetQualifier row as does TargetCompound.MZ for the target signal represented by the associated TargetCompound row given by CompoundID.

## MZExtractionWindowFilterLeft

[MZExtractionWindowFilterLeft](#) is the  $m/z$  value that controls the range on the left of the extracted  $m/z$  ion. The default value is 0.3.

## MZExtractionWindowFilterRight



[MZExtractionWindowFilterRight](#) the  $m/z$  value that controls the range on the right of the extracted  $m/z$  ion. The default value is 0.7.

# MZExtractionWindowUnits

[MZExtractionWindowUnitsLeft](#) represents the units used for [MZExtractionWindowFilterLeft](#) and [MZExtractionWindowFilterRight](#).

The units are the following:

- [Thomsons](#):

Thompson or m/z represents the physical quantity mass-to-charge ratio.

For example, the ion  $C_7H_7^{2+}$  an ion will be observed at 45.5 m/z

- PPM:

*Parts per million* ("ppm") denotes one particle of a given substance for every 999,999 other particles. One part in  $10^6$  — a precision of 0.0001%

The user can alternatively establish the mass extraction window value using ppm units.

$$\text{Ppm} = 10^6 * \Delta m \text{ accuracy} / m_{\text{measured}}$$

For example, at the theoretical mass of 1000 and a measured mass of 999.9 boundary is designated as 100 ppm.

- Percent:

*Percent* represents the mass extraction window as a percentage of the theoretical mass.

Enum Name	UI Name	Xpath expression
Thomsons	m/z	*//MZExtractionWindowUnits[.=' Thomsons `']
PPM	ppm	*//MZExtractionWindowUnits[.=' PPM' ]
Percent	Percent	*//MZExtractionWindowUnits[.=' Percent' ]

## OutlierPeakNotFound

[OutlierPeakNotFound](#) stores the flag that indicates qualifier peak is not found by integrator. If [enabled by default](#) or by applying Outlier Setup, an associated column is highlighted.

## PeakFilterThreshold

[PeakFilterThreshold](#) represents the type of threshold filter that is applied to the chromatogram peaks that were detected by the integrator. The choice of PeakFilterThreshold determines the interpretation of PeakFilterThresholdValue. The following choices of PeakFilterThreshold are available:

PeakFilterThreshold	Filter condition
PeakAreaAbsThreshold	Peaks with area less than PeakFilterThresholdValue are filtered out
PeakAreaPctThreshold (default)	Peaks whose area, divided by maximum peak area, is less than PeakFilterThresholdValue/100 are filtered out
PeakHeightAbsThreshold	Peaks with height less than PeakFilterThresholdValue are filtered out
PeakHeightPctThreshold	Peaks whose height, divided by maximum peak height, is less than PeakFilterThresholdValue/100 are filtered out

## PeakFilterThresholdValue

[PeakFilterThresholdValue](#) represents the threshold that is applied to the peak area or height, depending on the choice of PeakFilterThreshold. Chromatogram peaks that are below the PeakFilterThresholdValue are filtered out and are not considered as candidate peaks for quantitation.

## OutlierPeakNotFound

[OutlierPeakNotFound](#) stores the flag that indicates target qualifier peak is not found by integrator. If [enabled by default](#) or by applying Outlier Setup, an associated column is highlighted.

## QualifierName

[QualifierName](#) stores qualifier's metadata in terms of the CompoundName.

## QualifierRangeMaximum

[QualifierRangeMaximum](#) is the value stored after the qualifier ratio calculation. The qualifier range sets the upper limit for the qualifier ratio value. Thus, comparing the calculated qualifier ratio directly against this QualifierRangeMaximum determines if the qualifier falls within range.

## QualifierRangeMinimum

[QualifierRangeMinimum](#) is the value stored after the qualifier ratio calculation. The qualifier range sets the lower limit for the qualifier ratio value. Thus, comparing the calculated qualifier ratio directly against this QualifierRangeMinimum to determines if the qualifier falls within range.

## QuantitationMessage

[QuantitationMessage](#) records issues for a particular sample.

### **Example:**

If the qualifier signal is not present for a compound that requires a qualifier present, the QuantitationMessage records this issue.

## RelativeResponse

[RelativeResponse](#) expresses a nominal relative ratio of the integrator-determined responses of the signal for this TargetQualifier row versus the signal for the associated TargetCompound row. Default value is unity indicating that the response of the qualifier signal is equal to the response of its associated target signal.

## ScanType

[ScanType](#) represents a human-readable string describing the experimental technique used to collect the data used to analyze the chemical compound represented by this TargetQualifier row. Possible values include "MRM", "SRM", "Parent Ion Scan", or "Neutral Loss Scan". This string is subject to localization in other supported languages. If null, ScanType of parent quantifier is used.

<b>Enum Name</b>	<b>UI Name</b>	<b>XPath expression</b>
MRM	MRM	*//ScanType[.='MRM']
NeutralLoss	Neutral Loss	*//ScanType[.='NeutralLoss']
NeutralGain	Neutral Gain	*//ScanType[.='NeutralGain']
ProductIon	Product Ion	*//ScanType[.='ProductIon']
PrecursorIon	Precursor Ion	*//ScanType[.='PrecursorIon']
Ms1Scan	Ms1 Scan	*//ScanType[.='Ms1Scan']
Ms2Scan	Ms2 Scan	*//ScanType[.='Ms2Scan']
Ms1SIM	Ms1 SIM	*//ScanType[.='Ms1SIM']
Ms2SIM	Ms2 SIM	*//ScanType[.='Ms2SIM']

## SelectedMZ

[SelectedMZ](#) represents a mass-to-charge measurement, in units of daltons per unit charge, of the ions selected by the first-quadrupole stage in a tandem mass spectrometer used to perform this experiment.

The SelectedMZ sets the precursor ion in MS/MS scan type such as Multiple Reaction Monitoring (MRM) or Product Ion scan.

In MRM, the qualifier transition's precursor ion (SelectedMZ) is assigned as a different precursor ion than the Target transition's precursor ion.

For example,

- 335 -> 200 (Compound1 Target transition)
- 337 -> 200 (Compound1 Qualifier transition)

Often used to establish another qualifier transition utilizing the isotope ratio with compounds containing  $^{35}\text{Cl}$  /  $^{37}\text{Cl}$  or  $^{79}\text{Br}$  /  $^{81}\text{Br}$ .

## ThresholdNumberOfPeaks

[ThresholdNumberOfPeaks](#) is a maximum number of peaks found by the integrator.

## Transition

[Transition](#) represents a human-readable string that expresses the M/Z values measured for this compound. The format of the Transition string depends on ScanType. When ScanType = MRM, the transition string has the format "SelectedMZ -> MZ", where SelectedMZ is the precursor ion and MZ is the product ion.

## Uncertainty

[Uncertainty](#) is a value, which, along with the RelativeResponse column, defines tolerance bounds for the nominal qualifier ratio for this TargetQualifier row. UncertaintyRelativeOrAbsolute column determines whether the uncertainty is a percent of the RelativeResponse or an absolute margin.

### Example:

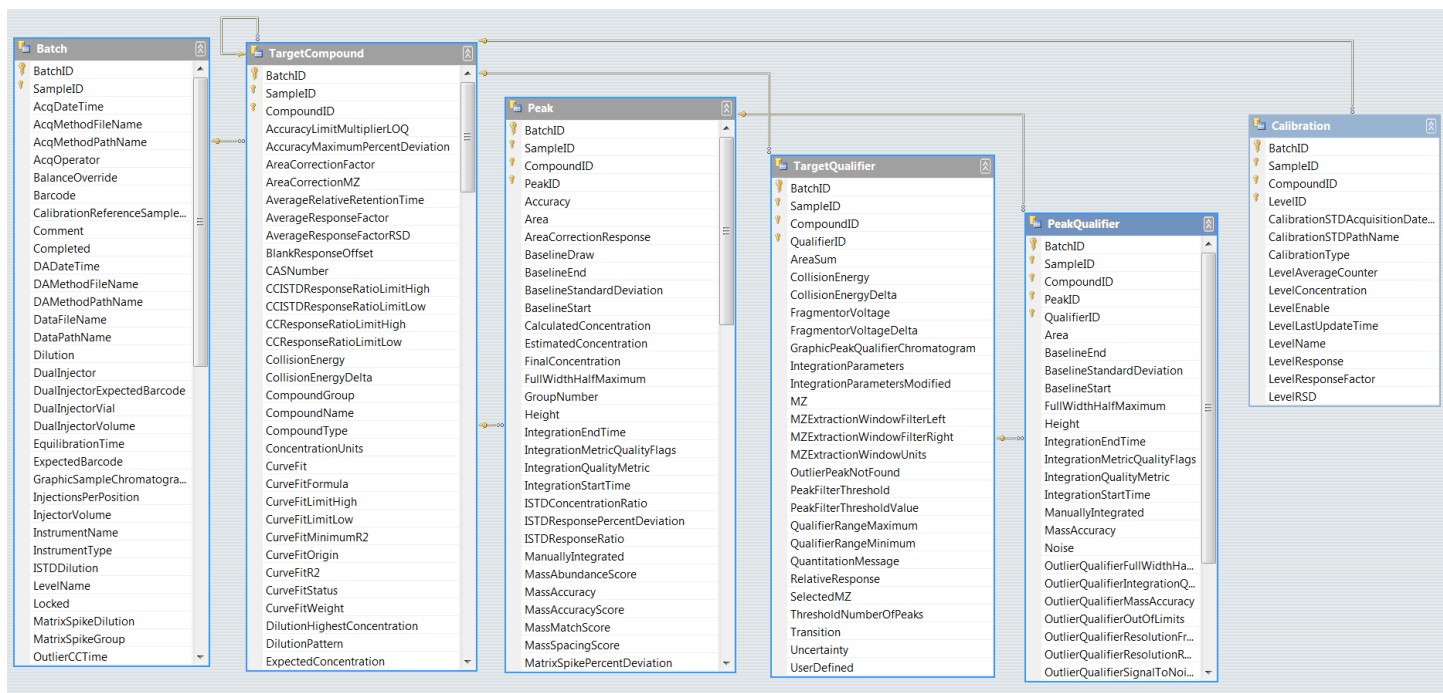
Consider a nominal qualifier signal ratio of 80 percent between Qualifier Q1 and this target compound, with a 20 per cent uncertainty. If UncertaintyRelativeOrAbsolute is 0, then the tolerance bounds for the qualifier ratio are 64 to 96, because 20 per cent of 80 is 16. If UncertaintyRelativeOrAbsolute is 1, then the tolerance bounds for the qualifier ratio are 60 to 100, because 20 per cent uncertainty is treated as an absolute offset from 80 per cent.

## UserDefined

[UserDefined](#) stores an arbitrary user-defined string.

UserDefined is editable in Batch-at-a-Glance.

# PeakQualifier Table



## Primary Key

{ [BatchID](#), [SampleID](#), [CompoundID](#), [PeakID](#), [QualifierID](#) } serves as the primary key. The composite of the [BatchID](#) and [SampleID](#) and [CompoundID](#) and [PeakID](#) and [QualifierID](#) and uniquely identify each row in this table. The keys in the Quantitation DataSet are not shown in the user interface.

A primary key value must be unique within the table. A composite key is a primary key that incorporates more than one column.

## BatchID

[BatchID](#) uniquely identifies the batch. [BatchID](#) is part of the composite primary key. The [BatchID](#) is typically set to -1 because Batch-at-a-Glance analyzes one batch.

## SampleID

[SampleID](#) uniquely identifies the sample in the batch. [SampleID](#) is part of the composite primary key. Thus, each sample in the batch is assigned a unique [SampleID](#).



## CompoundID

[CompoundID](#) uniquely identifies the sample in the batch. CompoundID is part of the composite primary key. Thus, each compound in the batch is assigned a unique CompoundID.

## PeakID

[PeakID](#) uniquely identifies the qualifier(s) for this compound. PeakID is part of the composite primary key.

Thus, each qualifier peak for this compound is assigned a unique PeakID.

## QualifierID

[QualifierID](#) uniquely identifies the qualifier(s) for this compound. QualifierID is part of the composite primary key. Thus, each qualifier for this compound is assigned a unique QualifierID.

## Area

[Area](#) contains the integrator-determined area of the peak represented by this PeakQualifier row.

## BaselineEnd

[BaselineEnd](#) is expressed in counts. Baseline represents the height of the trailing baseline endpoint.

## BaselineEndOriginal

[BaselineEndOriginal](#) records the BaselineEnd before performing manual integration.

## BaselineStandardDeviation

[BaselineStandardDeviation](#) stores an integration metric that measures the variation of the baseline.

## BaselineStart

[BaseLineStart](#) is expressed in counts. Baseline represents the height of the leading baseline endpoint.

Baseline regions are equivalent to noise regions only if the following two conditions hold:

1. the integrator provides the baseline region information
2. no user-defined regions are specified.

The parameterless integrators such as the Agile integrator provide baseline region information.

## BaselineStartOriginal

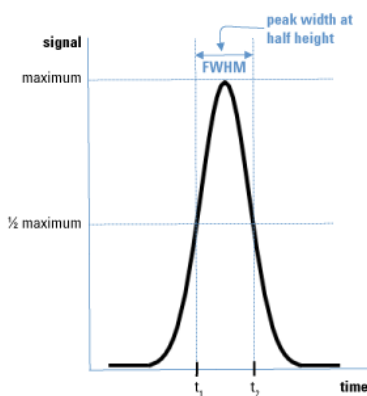
[BaselineStartOriginal](#) records the Baseline Start before performing manual integration.

## CoelutionScore

[CoelutionScore](#) is a measurement of how well this qualifier ion coelutes with the quantifier ion. The Coelution score uses the retention time of the quantifier ion and the quantifier ion as well as the peak width and the peak symmetry of the quantifier ion and the qualifier ion.

## FullWidthHalfMaximum

[FullWidthHalfMaximum](#) is the peak width at half height.



## Height

[Height](#) contains the integrator-determined height of the peak represented by this peak. Typically, Area is used as the measure of the size of the peak.

## IntegrationEndTime

[IntegrationEndTime](#) contains the integrator-determined peak-end chromatographic retention time value associated with the peak represented by this PeakQualifier row.

## IntegrationEndTimeOriginal

[IntegrationEndTimeOriginal](#) records the IntegrationEndTime before performing manual integration.

## IntegrationMetricQualityFlags

[IntegrationMetricQualityFlags](#) stores the reasons record by the MS-MS integrator.

- Based on several peak characteristics:
- Peak height
- Peak area
- Peak width
- Peak symmetry
- Merged peaks to the right or left
- Level of spikes on a peak

Enum Name	UI Name	Xpath expression
NoProblem	No Problem	<code>*//IntegrationMetricQualityFlags[.='NoProblem']</code>
InterferenceProblem	Interference Problem	<code>*//IntegrationMetricQualityFlags[.='InterferenceProblem']</code>
PeakArea	Peak area	<code>*//IntegrationMetricQualityFlags[.='PeakArea']</code>
WidthProblem	Width Problem	<code>*//IntegrationMetricQualityFlags[.='WidthProblem']</code>

Spiky	Spiky	*//IntegrationMetricQualityFlags[.='Spiky']
MergedProblem	Merged Problem	*//IntegrationMetricQualityFlags[.='MergedProblem']
SeriousProblem	Serious Problem	*//IntegrationMetricQualityFlags[.='SeriousProblem']

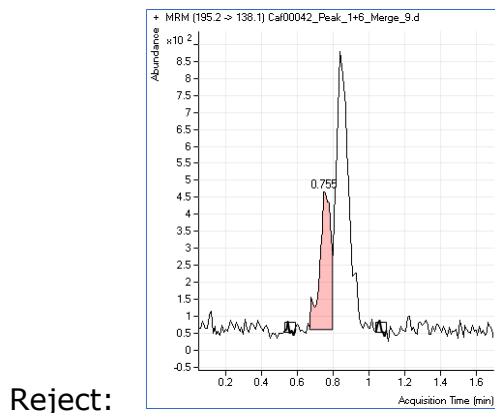
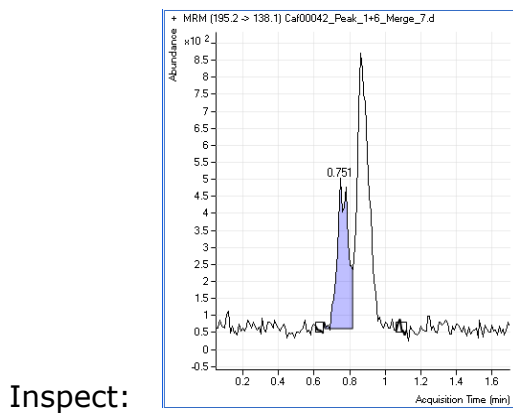
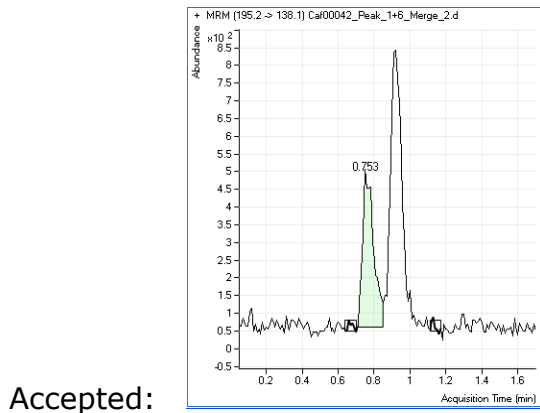
Note: the string of integrator problems can include multiple problem separated by commas.

For example: "WidthProblem, SeriousProblem"

# IntegrationQualityMetric

[IntegrationQualityMetric](#) stores the type of integration metric found by the MS-MS integrator. IntegrationQualityMetric relates to the [OutlierIntegrationQualityMetric](#).

IntegrationQualityMetric is classified the peak into categories:



Enum	UI Name	Xpath expression
------	---------	------------------

Name		
Accepted	Accepted	*//IntegrationQualityMetric[.='Accepted']
Inspect	Inspect	*//IntegrationQualityMetric[.='Inspect']
Rejected	Rejected	*//IntegrationQualityMetric[.='Rejected']

## IntegrationStartTime

[IntegrationStartTime](#) contains the integrator-determined peak-start chromatographic retention time value associated with the peak represented by this PeakQualifier row.

## IntegrationStartTimeOriginal

[IntegrationStartTimeOriginal](#) records the IntegrationStartTime before performing manual integration.

## ManuallyIntegrated

[ManuallyIntegrated](#) flag is true if and only if the integration results stored for this peak has been manually updated.

## MassAccuracy

[MassAccuracy](#) is the difference between the actual centroided spectral mass and expected MZ. It's measured in the unit as determined by the MZExtractionWindowUnits setting (Thomsons, PPM, Percent).

## MZ

[MZ](#) records the actual MZ used for mass accuracy calculation. In feature detection case, it is the feature assigned mass.

## NoiseRegions

[NoiseRegions](#) records the actual regions that are used for the noise calculation.

## OutlierQualifierCoelutionScore

[OutlierQualifierCoelutionScore](#) stores the flag resulting from this [outlier condition evaluation](#). If [enabled by default](#) or by applying Outlier Setup, an associated column is highlighted. See [Outlier Details](#).

## OutlierQualifierFullWidthHalfMaximum

[OutlierQualifierFullWidthHalfMaximum](#) stores the flag resulting from this [outlier condition evaluation](#). If [enabled by default](#) or by applying Outlier Setup, an associated column is highlighted. See [Outlier Details](#).

## OutlierQualifierIntegrationQualityMetric

[OutlierQualifierIntegrationQualityMetric](#) stores the flag resulting from this [outlier condition evaluation](#). If [enabled by default](#) or by applying Outlier Setup, an associated column is highlighted.

## OutlierQualifierMassAccuracy

[OutlierQualifierMassAccuracy](#) stores the flag resulting from this [outlier condition evaluation](#). If [enabled by default](#) or by applying Outlier Setup, an associated column is highlighted. See [Outlier Details](#).

## OutlierQualifierOutOfLimits

[OutlierQualifierOutOfLimits](#) stores the outlier flag for the [OutlierQualifierOutOfLimits](#).

## OutlierQualifierResolutionFront

[OutlierQualifierResolutionFront](#) stores the flag resulting from this [outlier condition evaluation](#). If [enabled by default](#) or by applying Outlier Setup, an associated column is highlighted. See [Outlier Details](#).

## OutlierQualifierResolutionRear

[OutlierQualifierResolutionRear](#) stores the flag resulting from this [outlier condition evaluation](#). If [enabled by default](#) or by applying Outlier Setup, an associated column is highlighted. See [Outlier Details](#).

## OutlierQualifierSignalToNoiseRatio

[OutlierQualifierSignalToNoiseRatio](#) stores the flag resulting from this [outlier condition evaluation](#). If [enabled by default](#) or by applying Outlier Setup, an associated column is highlighted. See [Outlier Details](#).

## OutlierQualifierSymmetry

[OutlierQualifierSymmetry](#) stores the outlier flag for the [OutlierQualifierOutOfLimits](#).

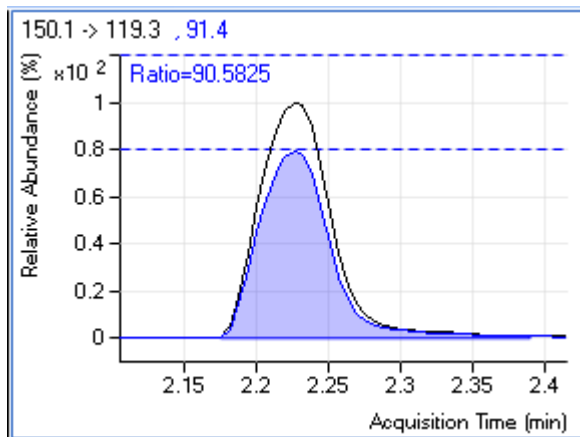
## OutlierSaturationRecovery

[OutlierSaturationRecovery](#) stores the flag resulting from the Saturation Recovery outlier condition evaluation. If [enabled by default](#) or by applying Outlier Setup, an associated column is highlighted.



## QualifierResponseRatio

[QualifierResponseRatio](#) sets the expected ratio between the target ion and its qualifier ion. For example, this ratio is typically measured to confirm the presence of a compound follows a certain fragmentation pattern.



## QualifierResponseRatioOriginal

[QualifierResponseRatioOriginal](#) records the [QualifierResponseRatio](#) before performing the manual integration.

## ResolutionFront

[ResolutionFront](#) is the chromatographic resolution of primary peak with the peak in front of it. It calculates the height of the valley between the peaks as a percent of the average height of the peaks.

## ResolutionRear

[ResolutionRear](#) is the chromatographic resolution of primary peak with the rear peak next to it. It calculates the height of the valley between the peaks as a percent of the average height of the peaks.

## RetentionTime

[RetentionTime](#) contains the integrator-determined peak-apex chromatographic retention time value associated with the peak represented by this PeakQualifier row.

## RetentionTimeOriginal

[RetentionTimeOriginal](#) records the Retention Time before performing manual integration.

## SaturationRecoveryRatio

[SaturationRecoveryRatio](#) represents the ratio of the restored feature peak height to the original feature peak height. The feature peak and recovery of feature peak are determined by the feature detection algorithm for accurate mass data.

Saturation Recovery Ratio	Recovery Status
Null	Feature is not saturated
0	Feature is saturated and not recovered
>0	Feature is saturated but recovered

## SignalToNoiseRatio

[SignalToNoiseRatio](#) represents the ratio of the signal to noise based on the [NoiseAlgorithmType](#) for each peak that identifies a compound amount. The S/N ratio is typically measures a significance of the signal strength above the noise.

## Symmetry

[Symmetry](#) represents the balance between the back and front of the peak. Symmetry of 1.0 means the peak is balanced. Smaller numbers less than one indicate asymmetry and peak fronting whereas larger numbers indicate peak tailing.

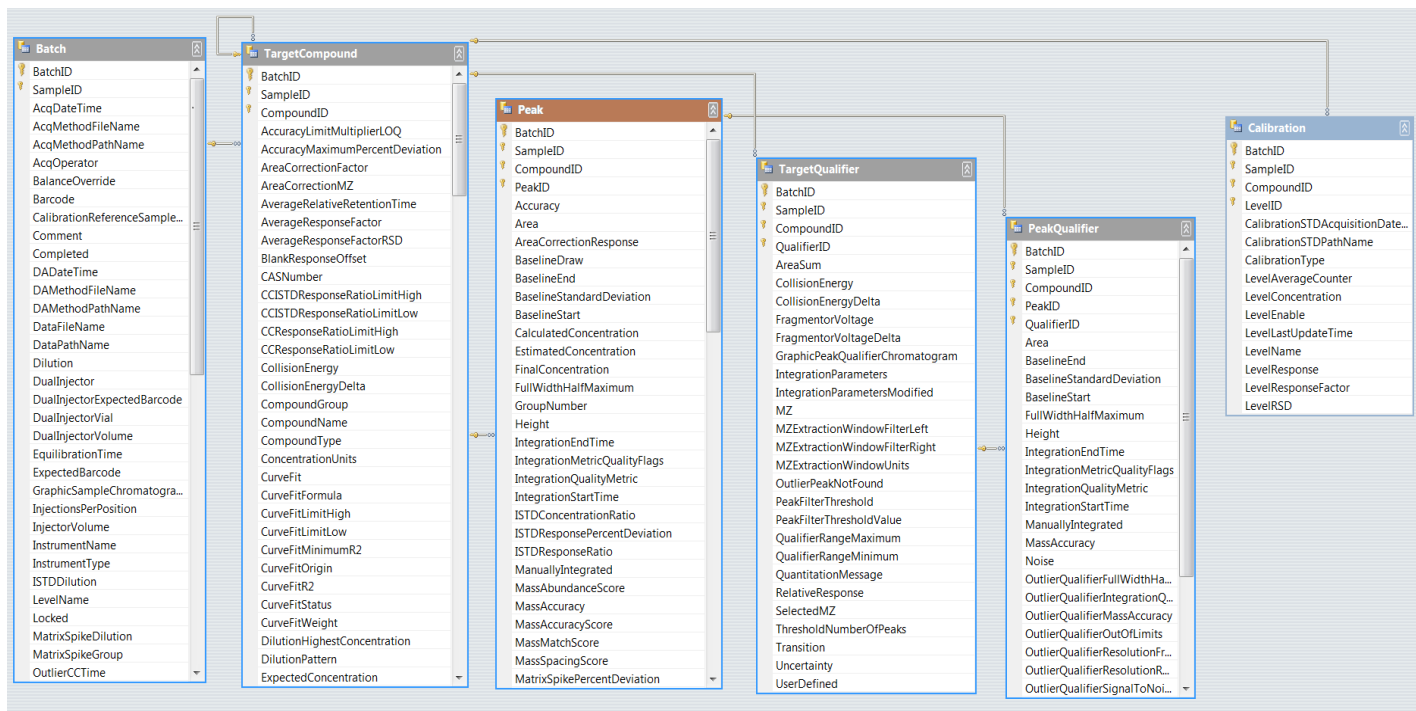
Symmetry = Distance (tail) / Distance (front)

# UserCustomCalculation

[UserCustomCalculation](#) stores a result from a custom calculation.

UserCustomCalculation work with an undocumented scripting mechanism.

# Peak Table



## Primary Key

{ [BatchID](#), [SampleID](#), [CompoundID](#), [PeakID](#) } serves as the primary key. The composite of the [BatchID](#) and [SampleID](#) and [CompoundID](#) and [PeakID](#) and unique identify each row in this table. The keys in the Quantitation DataSet are not show in the user interface.

A primary key value must be unique with in the table. A composite key is a primary key that incorporates more than one column.

## BatchID

[BatchID](#) uniquely identifies the batch. [BatchID](#) is part of the composite primary key. The [BatchID](#) is typically set to -1 because Batch-at-a-Glance analyzes one batch.

## SampleID

[SampleID](#) uniquely identifies the sample in the batch. [SampleID](#) is part of the composite primary key. Thus, each sample in the batch is assigned a unique [SampleID](#).

# CompoundID

[CompoundID](#) uniquely identifies the sample in the batch. CompoundID is part of the composite primary key. Thus, each compound in the batch is assigned a unique CompoundID.

# PeakID

[PeakID](#) uniquely identifies the peak(s) for this compound. PeakID is part of the composite primary key.

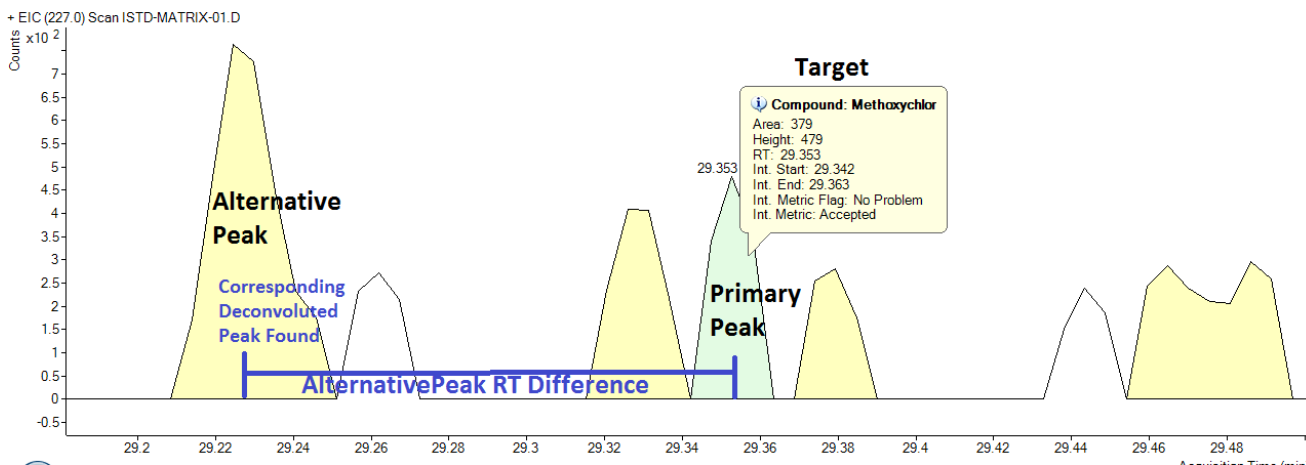
Thus, each peak for this compound is assigned a unique PeakID.

# Accuracy

[Accuracy](#) gives the relative error of the computed concentration versus the expected concentration.

# AlternativePeakRTDiff

[AlternativePeakRTDiff](#) is the RT difference between the primary peak and the better alternative peak identified by the [AlternativePeakCriteria](#).



Alternative Deconvoluted Peak LMS is better than Target Peak deconvoluted LMS, matching against Target reference.

# AlternativeTargetHit

AlternativeTargetHit is only reported when a Target peak is Found AND Target Deconvoluted (TD) peak is Found. Alternative Hit demonstrates NIST search result. The search result is shown

as string which can be further parsed by report, the format of the string is { TargetRank; NIST LMS for target compound; Top NIST hit CompoundName; Top NIST hit CAS#; Top NIST hit LMS; library Compound ID; library Spectrum ID }. Library Compound ID and Library Spectrum ID are used by reporting system to retrieve compound library spectrum.

## Area

[Area](#) represents the integrator-determined area of the peak represented by this Peak row.

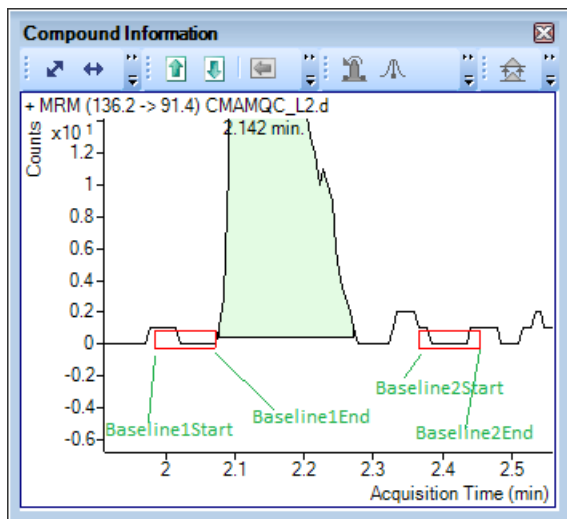
## AreaCorrectionResponse

[AreaCorrectionResponse](#) is the product of the integrated area of the area correction signal and the area correction factor, as specified in the associated TargetCompound row. If the area correction signal is `NULL` in the associated TargetCompound row, then AreaCorrectionResponse is zero.

## BaselineDraw

[BaselineDraw](#) contains graphics information used to draw the baseline calculation points for a peak.

This value consists of 5 numbers: Baseline1Start, Baseline1End, Baseline2Start, Baseline2End, BaselineOffset. They are illustrated in the figure below. BaselineOffset is Y coordinate of the middle of the boxes. [BaselineStandardDeviation](#) is height of the boxes.



## BaselineEnd

[BaselineEnd](#) is expressed in counts. It represents the height of the trailing baseline endpoint.

## BaselineEndOriginal

[BaselineEndOriginal](#) records the BaselineEnd before performing manual integration.

## BaselineStandardDeviation

[BaselineStandardDeviation](#) is a metric calculated for all parameterless integrators: MS-MS, MS-MS (GC), and Agile.

## BaselineStart

[BaselineStart](#) is expressed in counts. It represents the height of the leading baseline endpoint.

## BaselineStartOriginal

[BaselineStartOriginal](#) records the Baseline Start before performing manual integration.



## CalculatedConcentration

[CalculatedConcentration](#) is expressed in the units given by the ConcentrationUnits value in the associated TargetCompound row. It indicates the concentration value calculated by the quantitation algorithm for the peak represented by this Peak row.

## CapacityFactor

[CapacityFactor](#) is a measure of the retention of a peak that is independent of column geometry or mobile phase flow rate. It is the ratio of the amount of time a solute spends in the stationary and mobile phases. For example, a solute with a  $k' = 6$  is twice as retained by the stationary phase (but not the column) as a solute with a  $k' = 3$ . The capacity factor does not provide absolute retention information; it provides relative retention information. An unretained compound has a capacity factor of 0.  $T_r$  is the retention time.  $T_o$  is the retention time of an unretained compound. The equation is

$$(T_r - T_o) / T_o$$

## CCISTDResponseRatio

[CCISTDResponseRatio](#) stores ISTD response deviation in any sample type from the most recent Continuing Calibration sample.

## CCResponseRatio

[CCResponseRatio](#) stores the compound's CC response ratio to the initial calibration at the same calibration level.

## EstimatedConcentration

[EstimatedConcentration](#) stores a range that estimates the concentration of a tentatively identified compound after Unknowns Analysis.

re

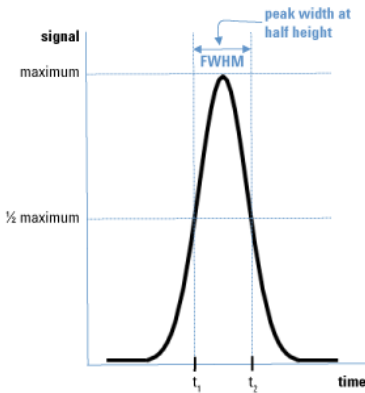
Typically, the range is derived from the averaged response factor of all the target compounds. The estimate is typically within an order of magnitude.

## FinalConcentration

[FinalConcentration](#) is the typically the amount reported for this sample's compound.

## FullWidthHalfMaximum

[FullWidthHalfMaximum](#) is the peak width at half height.



## GroupNumber

[GroupNumber](#) is an integer that uniquely identifies the signal-correlation-algorithm peak-group within the space of all peaks collected to analyze the associated TargetCompound. The peak group for this Peak row is comprised of its peak and its associated PeakQualifier rows' peaks.

## Height

[Height](#) contains the integrator-determined height of the peak represented by this Peak row.

## IntegrationEndTime

[IntegrationEndTime](#) contains the integrator-determined peak-end chromatographic retention time value associated with the peak represented by this Peak row.

## IntegrationEndTimeOriginal

[IntegrationEndTimeOriginal](#) records the IntegrationEndTime before performing manual integration.

## IntegrationMetricQualityFlags

[IntegrationMetricQualityFlags](#) stores the reasons record by the MS-MS integrator.

Based on several peak characteristics:

- Peak height
- Peak area
- Peak width
- Peak symmetry
- Merged peaks to the right or left
- Level of spikes on a peak

## IntegrationStartTime

[IntegrationStartTime](#) contains the integrator-determined peak-start chromatographic retention time value associated with the peak represented by this Peak row.

## IntegrationStartTimeOriginal

[IntegrationStartTimeOriginal](#) records the IntegrationStartTime before performing manual integration.

## ISTDConcentrationRatio

[ISTDConcentrationRatio](#) is used whenever the peak represented by this Peak row is related to an internal-standard peak, and in that case is the ratio of the computed concentrations for this peak and that of the internal standard peak. Wherever this peak is not related to an internal-standard peak, this value is undefined.

## ISTDResponsePercentDeviation

[ISTDResponsePercentDeviation](#) is the deviation of a compound's internal standard response (area or height) from the average ISTD response calculated from the existing calibration.

## ISTDResponseRatio

[ISTDResponseRatio](#) is used whenever the peak represented by this Peak row is related to an internal-standard peak, and in that case is the ratio of the determined responses for this peak and that of the internal standard peak. Wherever this peak is not related to an internal-standard peak, this value is undefined.

The ISTDResponseRatio is adjusted to take into account isotope ratios.

## ManuallyIntegrated

[ManuallyIntegrated](#) flag is true if and only if the integration results stored for this peak have been manually updated.

## MassAbundanceScore

[MassAbundanceScore](#) is the calculated comparison of the mass abundance in the actual spectrum compared to the normalized mass abundance ratios of synthesized spectral pattern.

## MassAccuracy

[MassAccuracy](#) is the difference between the actual centroided spectral mass and expected MZ. It's measured in the unit as determined by the MZExtractionWindowUnits setting (Dalton, PPM, Percent).

## MassAccuracyScore

[MassAccuracyScore](#) is the calculated comparison of the mass accuracy in the actual spectrum compared to the mass accuracy of synthesized spectral pattern.

## MassMatchScore

[MassMatchScore](#) is the weighted aggregate of the individual metrics calculated when comparing an actual spectrum with a spectrum pattern synthesized from a formula.

## MassSpacingScore

[MassSpacingScore](#) is the calculated comparison of the mass isotopic spacing in the actual spectrum compared to the mass isotopic spacing of synthesized spectral pattern.

## MatrixSpikePercentRecovery

[MatrixSpikePercentRecovery](#) is a value calculated in the [OutlierMatrixSpikePercentRecovery](#).

## MatrixSpikePercentDeviation

[MatrixSpikePercentDeviation](#) is a value calculated in the [OutlierMatrixSpikePercentDeviation](#).

## MZ

[MZ](#) records the actual MZ used for mass accuracy calculation. In feature detection case, it is the feature assigned mass.

## Noise

[Noise](#) is calculated based on the selected [NoiseAlgorithmType](#) for each peak that identifies a compound amount.

## NoiseRegions

[NoiseRegions](#) records the actual regions that are used for the noise calculation.

## NumberOfVerifiedIons

[NumberOfVerifiedIons](#) is calculated based on the number of qualifier ions and quantifier that meet the SANTE criteria, i.e., no mass accuracy outlier, no S/N outlier and no coelution score outlier.

## OutlierAccuracy

[OutlierAccuracy](#) stores the flag resulting from this [outlier condition evaluation](#). If [enabled by default](#) or by applying Outlier Setup, an associated column is highlighted.

## OutlierBelowLimitOfDetection

[OutlierBelowLimitOfDetection](#) stores the flag resulting from this [outlier condition evaluation](#). If [enabled by default](#) or by applying Outlier Setup, an associated column is highlighted. See [Outlier Details](#).

## OutlierBelowLimitOfQuantitation

[OutlierBelowLimitOfQuantitation](#) stores the flag resulting from this [outlier condition evaluation](#). If [enabled by default](#) or by applying Outlier Setup, an associated column is highlighted.



## OutlierBlankConcentrationOutsideLimit

[OutlierBlankConcentrationOutsideLimit](#) stores the flag resulting from this [outlier condition evaluation](#). If [enabled by default](#) or by applying Outlier Setup, an associated column is highlighted. See [Outlier Details](#).

## OutlierCapacityFactor

[OutlierCapacityFactor](#) stores the flag resulting from this [outlier condition evaluation](#). If [enabled by default](#) or by applying Outlier Setup, an associated column is highlighted. See [Outlier Details](#).

## OutlierCCISTDResponseRatio

[OutlierCCISTDResponseRatio](#) stores the flag resulting from this [outlier condition evaluation](#). If [enabled by default](#) or by applying Outlier Setup, an associated column is highlighted. See [Outlier Details](#).

## OutlierCCResponseRatio

[OutlierCCResponseRatio](#) stores the flag resulting from this [outlier condition evaluation](#). If [enabled by default](#) or by applying Outlier Setup, an associated column is highlighted. See [Outlier Details](#).

## OutlierCCRetentionTime

[OutlierCCRetentionTime](#) stores the flag resulting from this [outlier condition evaluation](#). If [enabled by default](#) or by applying Outlier Setup, an associated column is highlighted. See [Outlier Details](#).

## OutlierFullWidthHalfMaximum

[OutlierFullWidthHalfMaximum](#) stores the flag resulting from this [outlier condition evaluation](#). If [enabled by default](#) or by applying Outlier Setup, an associated column is highlighted. See [Outlier Details](#).

## OutlierLibraryMatchScore



[OutlierLibraryMatchScore](#) stores the flag resulting from this [outlier condition evaluation](#). If [enabled by default](#) or by applying Outlier Setup, an associated column is highlighted. See [Outlier Details](#).

## OutlierMassAccuracy

[OutlierMassAccuracy](#) stores the flag resulting from this [outlier condition evaluation](#). If [enabled by default](#) or by applying Outlier Setup, an associated column is highlighted. See [Outlier Details](#).

## OutlierMassMatchScore

[OutlierMassMatchScore](#) stores the flag resulting from this [outlier condition evaluation](#). If [enabled by default](#) or by applying Outlier Setup, an associated column is highlighted. See [Outlier Details](#).

## OutlierMatrixSpikeGroupRecovery

[OutlierMatrixSpikeGroupRecovery](#) stores the flag resulting from this [outlier condition evaluation](#). If [enabled by default](#) or by applying Outlier Setup, an associated column is highlighted. See [Outlier Details](#).

## OutlierNumberOfQualifiedIons

[OutlierNumberOfQualifiedIons](#) stores the flag resulting from this [outlier condition evaluation](#). If [enabled by default](#) or by applying Outlier Setup, an associated column is highlighted. See [Outlier Details](#).

## OutlierOutOfCalibrationRange

[OutlierOutOfCalibrationRange](#) stores the flag resulting from this [outlier condition evaluation](#). If [enabled by default](#) or by applying Outlier Setup, an associated column is highlighted. See [Outlier Details](#).

## OutlierPlates

[OutlierPlates](#) stores the flag resulting from this [outlier condition evaluation](#). If [enabled by default](#) or by applying Outlier Setup, an associated column is highlighted. See [Outlier Details](#).

## OutlierQValue

[OutlierQValue](#) stores the flag resulting from this [outlier condition evaluation](#). If [enabled by default](#) or by applying Outlier Setup, an associated column is highlighted. See [Outlier Details](#).

## OutlierIntegrationQualityMetric

[OutlierIntegrationQualityMetric](#) stores the flag resulting from this [outlier condition evaluation](#). If [enabled by default](#) or by applying Outlier Setup, an associated column is highlighted. See [Outlier Details](#).

## OutlierISTDResponse

[OutlierISTDResponse](#) stores the flag resulting from this [outlier condition evaluation](#). If [enabled by default](#) or by applying Outlier Setup, an associated column is highlighted. See [Outlier Details](#).

## OutlierISTDResponsePercentDeviation

[OutlierISTDResponsePercentDeviation](#) stores the flag resulting from this [outlier condition evaluation](#). If [enabled by default](#) or by applying Outlier Setup, an associated column is highlighted. See [Outlier Details](#).

## OutlierMatrixSpikeOutOfLimits

[OutlierMatrixSpikeOutOfLimits](#) stores the flag resulting from this [outlier condition evaluation](#). If [enabled by default](#) or by applying Outlier Setup, an associated column is highlighted. See [Outlier Details](#).

## OutlierMatrixSpikeOutsidePercentDeviation

[OutlierMatrixSpikeOutsidePercentDeviation](#) stores the flag resulting from this [outlier condition evaluation](#). If [enabled by default](#) or by applying Outlier Setup, an associated column is highlighted.

## OutlierMatrixSpikePercentRecovery

[OutlierMatrixSpikePercentRecovery](#) stores the flag resulting from this [outlier condition evaluation](#). If [enabled by default](#) or by applying Outlier Setup, an associated column is highlighted. See [Outlier Details](#).

## OutlierPurity

[OutlierPurity](#) stores the flag resulting from this [outlier condition evaluation](#). If [enabled by default](#) or by applying Outlier Setup, an associated column is highlighted. See [Outlier Details](#).

## OutlierQCLCSRecoveryOutOfLimits

[OutlierQCLCSRecoveryOutOfLimits](#) stores the flag resulting from this [outlier condition evaluation](#). If [enabled by default](#) or by applying Outlier Setup, an associated column is highlighted. See [Outlier Details](#).

## OutlierQCOutOfLimits

[OutlierQCOutOfLimits](#) stores the flag resulting from this [outlier condition evaluation](#). If [enabled by default](#) or by applying Outlier Setup, an associated column is highlighted. See [Outlier Details](#).

## OutlierQCOutsideRSD

[OutlierQCOutsideRSD](#) stores the flag resulting from this [outlier condition evaluation](#). If [enabled by default](#) or by applying Outlier Setup, an associated column is highlighted. See [Outlier Details](#).

## OutlierRelativeRetentionTime

[OutlierRelativeRetentionTime](#) stores the flag resulting from this [outlier condition evaluation](#). If [enabled by default](#) or by applying Outlier Setup, an associated column is highlighted. See [Outlier Details](#).

## OutlierResolutionFront

[OutlierResolutionFront](#) stores the flag resulting from this [outlier condition evaluation](#). If [enabled by default](#) or by applying Outlier Setup, an associated column is highlighted. See [Outlier Details](#).

## OutlierResolutionRear

[OutlierResolutionRear](#) stores the flag resulting from this [outlier condition evaluation](#). If [enabled by default](#) or by applying Outlier Setup, an associated column is highlighted. See [Outlier Details](#).

## OutlierRetentionTime

[OutlierRetentionTime](#) stores the flag resulting from this [outlier condition evaluation](#). If [enabled by default](#) or by applying Outlier Setup, an associated column is highlighted. See [Outlier Details](#).

## OutlierSampleAmountOutOfLimits

[OutlierSampleAmountOutOfLimits](#) stores the flag resulting from this [outlier condition evaluation](#). If [enabled by default](#) or by applying Outlier Setup, an associated column is highlighted. See [Outlier Details](#).

## OutlierSampleOutsideRSD

[OutlierSampleOutsideRSD](#) stores the flag resulting from this [outlier condition evaluation](#). If [enabled by default](#) or by applying Outlier Setup, an associated column is highlighted. See [Outlier Details](#).

## OutlierSignalToNoiseRatioBelowLimit

[OutlierSignalToNoiseRatioBelowLimit](#) stores the flag resulting from this [outlier condition evaluation](#). If [enabled by default](#) or by applying Outlier Setup, an associated column is highlighted. See [Outlier Details](#).

## OutlierSurrogateOutOfLimits

[OutlierSurrogateOutOfLimits](#) stores the flag resulting from this [outlier condition evaluation](#). If [enabled by default](#) or by applying Outlier Setup, an associated column is highlighted. See [Outlier Details](#).

## OutlierSurrogatePercentRecovery

[OutlierSurrogatePercentRecovery](#) stores the flag resulting from this [outlier condition evaluation](#). If [enabled by default](#) or by applying Outlier Setup, an associated column is highlighted. See [Outlier Details](#).

## OutlierSymmetry

[OutlierSymmetry](#) stores the flag resulting from this [outlier condition evaluation](#). If [enabled by default](#) or by applying Outlier Setup, an associated column is highlighted. See [Outlier Details](#).

## Plates

The number of theoretical plates of the column efficiency. Theoretical plates is a concept and a column does not contain anything resembling physical distillation plates or any other similar feature. Theoretical plates numbers are an indirect measure of peak width for a peak at a specific retention time. Columns with high plate numbers are considered to be more efficient (higher column efficiency) than columns with lower plate numbers. A column with a high number of plates will have a narrower peak at a given retention time than a column with a lower number of plates.

Different pharmacopeia uses different formulas to determine the value for Plates.

Pharmacopeia	Formula
Default	$16 * (Tr / Wb) ^2$
USP	$16 * (Tr / Wb) ^2$
EU	$5.54 * (Tr / W50) ^2$
JP	$5.54 * (Tr / W50) ^2$

Tr is the retention time

Wb is the peak width determine by the tangent method.

W50 is the peak width at 50% of the height of the peak.

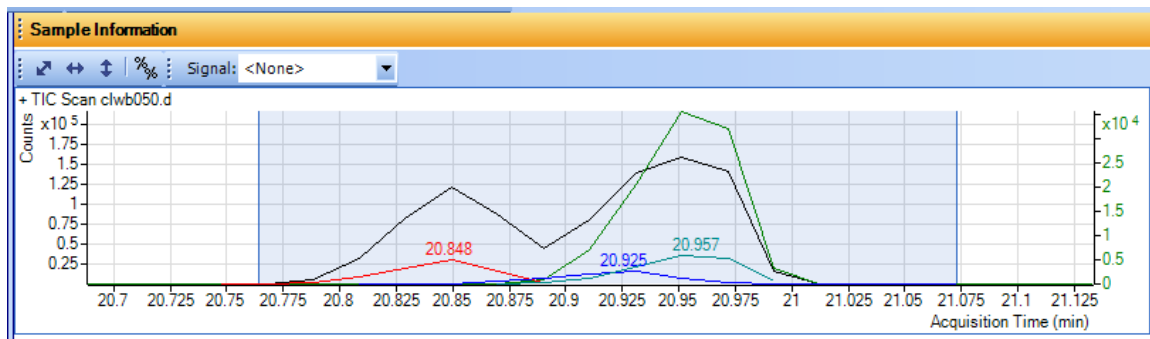
Theoretical plate numbers are only valid for a specific set of conditions. Isothermal temperature conditions are required and temperature programs result in highly inflated plate numbers. When comparing theoretical plate numbers between columns, the same temperature conditions and peak retention ( $k'$ ) are required for the comparison to be valid.

## PromoteHit

[PromoteHit](#) stores user's manual choice for the screening result. User can change among three screening result categories: "positive" "warning" and "negative".

## Purity

[Purity](#) aka Peak Purity estimates the percentage of the component ions from the spectra that group together and constitute the target relative to other components present.



**Peak Purity 1: Spectral deconvolution estimates the “purity” of the compound by evaluating other co-eluting spectral signals.**

Diagram shows a visualization of the components resulting from applying a deconvolution algorithm to the mass spectrometric scan data.

The purity calculation entails running a deconvolution on the entire chromatographic range of the sample. However, the new algorithm differs from the previously released versions (prior to B.05.02) in several important aspects:

- 1) The identification of the component that matches the target compound (the “target component”) uses a different set of criteria that makes it more robust:
  - a. For each component found by deconvolution, the system finds all component spectrum peaks that fall within the  $m/z$  delta range of the target quantifier  $m/z$ .
  - b. For every such component spectrum peak, the system checks if the corresponding ion peak (EIC peak) has an apex within the RT range of the target quantifier peak.
  - c. The component with the largest such peak is identified as the target component.
- 2) If the system fails to find a target component for any given target compound, it re-tries by running the full-sample deconvolution in “high-resolution” mode, using a window size factor that is reduced by a factor of 2. The high-resolution results are cached and are searched for any target compound that cannot be found in the normal-resolution component list. The automatic generation of the high-resolution results allows many target components to be identified that were previously missed.
- 3) The system attempts to detect “double components” that share the same RT and base peak  $m/z$ . The presence of such component doublets can strongly bias the purity estimate to the downside. Component doublets can occur if the RT window size factor is too small. Therefore, the system attempts to recover automatically by re-running the full-sample deconvolution in “low-resolution” mode, using a window size factor that is increased by a factor of 2. The low-resolution results are cached and are searched for any target that is matched to a component doublet.
- 4) The new purity calculation uses a different formula that gives more meaningful results in cases of severe interference. (The old purity definition can yield zero purity for such cases.) The new definition of purity uses the following formula:

$$\text{Purity}(\text{Target compound}) = \text{Area}(\text{Target component shape}) / \text{SUM}(\text{Area}(\text{Contributing component shape}))$$



The SUM is over all contributing components. A contributing component is any component that has spectral peaks within m/z delta range of the target quantifier m/z and overlaps the target peak in retention time.

## QvalueComputed

[QvalueComputed](#) contains a correlation statistic called QVALUE which measures the fidelity of the observed qualifier ratios versus the nominal qualifier ratios. The QVALUE function is a well-defined statistic that yields an efficient measure of the "goodness of fit" of the observed qualifier ratios to the nominal qualifier ratios.

For all hits a QVALUE is computed as described here. For Target Compound Entries with no qualifier signals, the QVALUE is defined as 100. For Target Compound Entries with k qualifier signals  $q_i$ ,  $1 \leq i \leq k$ , define  $r_i$  as the expected ratio of qualifier peak for  $q_i$  to the target peak. Then define  $r_i'$  as the observed qualifier ratio as determined by the above Qualifier Ratio Computation. Now define the total ratio deviation D:

$$D = \frac{\sum_{1 \leq i \leq k} (100|r_i - r_i'|) (\ln(100r_i + 1))^2}{21.3 \sum_{1 \leq i \leq k} r_i}$$

Then the QVALUE is the closest integer to  $\max \{ 100 - D, 1 \}$ .

## QvalueSort

[QvalueSort](#) is equal to QvalueComputed unless the PeakSelectionCriterion for the associated TargetCompound is Greatest Response or Closest Retention Time, in which case it is zero.

## ReferenceLibraryMatchScore

[ReferenceLibraryMatchScore](#) records the measure of the correlation between the spectrum and the reference library spectrum, or in the case of "Target Deconvolution", between deconvoluted spectrum and the reference library spectrum. The reference library can be generated from a high level calibration sample or from an existing library.

ReferenceLibraryMatchScore is an indicator of the quality of the match between the sample spectrum and the reference library spectrum. A score of 100 means a perfect match.

## RelativeRetentionTime

[RelativeRetentionTime](#) represents the ratio of the target compound's retention time to the related ISTD's retention time. RelativeRetentionTime is a value used in calculation of [OutlierRelativeRetentionTime](#).

# ResolutionFront

[ResolutionFront](#) is the chromatographic resolution of primary peak with the peak in front of it (left peak). Different pharmacopeia uses different formulas to determine the value for Resolution.

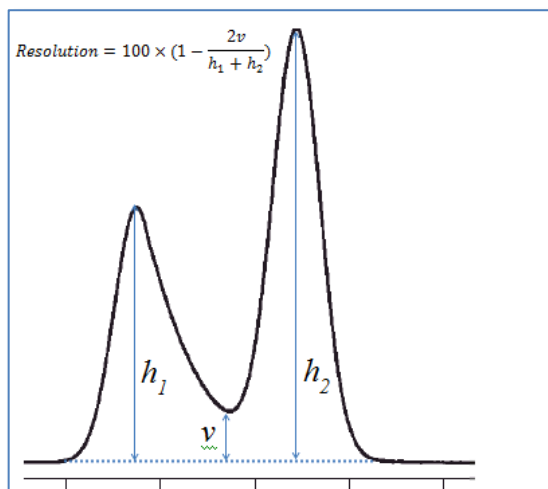
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## Pharmacopeia

## Formula

---

Default



USP

$$2 * (Tr,2 - Tr,1) / (Wb,1 + Wb,2)$$

EU

$$1.18 * (Tr,2 - Tr,1) / (W50,1 + W50,2)$$

JP

$$1.18 * (Tr,2 - Tr,1) / (W50,1 + W50,2)$$

Valley Height/Peak Height

$$v/h_2$$

Valley Height/Peak Height  
Average

$$100 * \frac{2v}{h_1 + h_2}$$

Valley Height/Peak Height  
Sum

$$100 * \frac{v}{h_1 + h_2}$$

- 
- $Tr,2$  is the retention time of the right peak in the peak pair.
  - $Tr,1$  is the retention time of the left peak in the peak pair.
  - Sigma is half the peak width at inflection points.
  - $Wb$  is the peak width determine by the tangent method.
  - $W50$  is the peak width at 50% of the height of the peak.

# ResolutionRear

[ResolutionRear](#) is the chromatographic resolution of primary peak with the rear peak next to it (right peak). Different pharmacopeia uses different formulas to determine the value for Resolution.

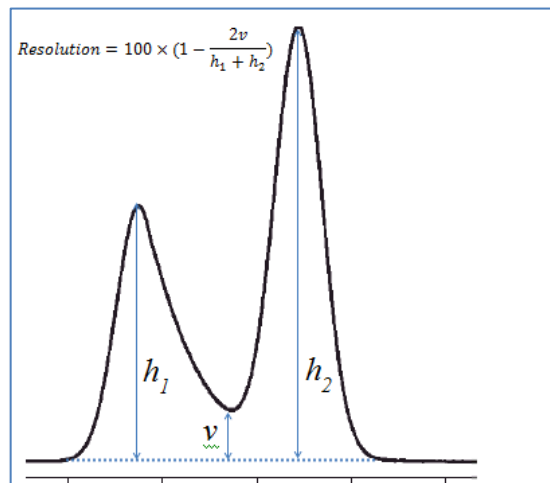
---

## Pharmacopeia

## Formula

---

Default



USP

$$2 * (Tr,2 - Tr,1) / (Wb,1 + Wb,2)$$

EU

$$1.18 * (Tr,2 - Tr,1) / (W50,1 + W50,2)$$

JP

$$1.18 * (Tr,2 - Tr,1) / (W50,1 + W50,2)$$

Valley Height/Peak Height

$$v/h_1$$

Valley Height/Peak Height  
Average

$$100 * \frac{2v}{h_1 + h_2}$$

Valley Height/Peak Height  
Sum

$$100 * \frac{v}{h_1 + h_2}$$


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- $Tr,2$  is the retention time of the right peak in the peak pair.
- $Tr,1$  is the retention time of the left peak in the peak pair.
- Sigma is half the peak width at inflection points.
- $Wb$  is the peak width determine by the tangent method.
- $W50$  is the peak width at 50% of the height of the peak.

## ResponseOriginal

[ResponseOriginal](#) records the target response before performing manual integration.

## ResponseRatio

[ResponseRatio](#) is used whenever the peak represented by this Peak row is related to an internal-standard peak, and in that case is the ratio of the determined responses for this peak and that of the internal standard peak. Wherever this peak is not related to an internal-standard peak, this value is undefined.

## RetentionIndex

[RetentionIndex](#) is calculated from the RT calibration file specified in the library method. The RTCalibration stores an array of RT/RI points which are used with Retention Indices.

## RetentionTime

[RetentionTime](#) contains the integrator-determined peak-apex chromatographic retention time value associated with the peak represented by this Peak row.

## RetentionTimeDifference

[RetentionTimeDifference](#) is expressed in minutes. RetentionTimeDifference gives the difference between the expected retention time of the target (possibly corrected for internal-standard retention time) and the SelectedGroupRetentionTime of this Peak row.

## RetentionTimeDifferenceKey

[RetentionTimeDifferenceKey](#) is expressed in millisecond. Its value depends on the PeakSelectionCriterion value in the associated TargetCompound. Whenever the PeakSelectionCriterion is not Greatest Peak Response, RetentionTimeDifferenceKey is the absolute value of RetentionTimeDifference. Otherwise it is zero.

## RetentionTimeOriginal

[RetentionTimeOriginal](#) records the Retention Time before performing manual integration.

## SampleRSD

[SampleRSD](#) is the relative standard deviation (RSD) of the final concentration for all samples of the same [SampleGroup](#) and of sample type Sample in the batch. If [SampleGroup](#) is not assigned, RSD for all samples of the sample type Sample in the batch is calculated.

## SaturationRecoveryRatio

[SaturationRecoveryRatio](#) represents the ratio of the restored feature peak height to the original feature peak height. The feature peak and recovery of feature peak are determined by the feature detection algorithm for accurate mass data.

Saturation Recovery Ratio = null => Feature is **Not Saturated**

Saturation Recovery Ratio != null => Feature is **Saturated**

Saturation Recovery Ratio == 0 => Feature is **Saturated and not recovered**

Saturation Recovery Ratio > 0 => Feature is **Saturated but recovered**

## SelectedGroupRetentionTime

[SelectedGroupRetentionTime](#) contains the aggregate (average) retention time assigned to the peak group containing this peak during the application of the signal-correlation algorithm to the set of peaks (containing this peak and its associated PeakQualifier peaks). The details of the signal-correlation algorithm are beyond the scope of this document.

## SelectedTargetRetentionTime

[SelectedTargetRetentionTime](#) contains the retention time assigned to this peak by the integration algorithm.

## SignalToNoiseRatio

[SignalToNoiseRatio](#) represents the strength of the signal. SignalToNoiseRatio is calculated by several different algorithms set by [NoiseAlgorithmType](#). Refer to Qualitative Analysis documentation for further details.

## SurrogatePercentRecovery

[SurrogatePercentRecovery](#) is a value used in the calculation of the [OutlierSurrogatePercentRecovery](#).

## Symmetry

[Symmetry](#) represents the balance between the back and front of the peak. Symmetry of 1.0 means the peak is balanced. Smaller numbers than one indicate asymmetry and peak fronting. Larger numbers than one indicate asymmetry and peak fronting.

Symmetry = Distance (tail) / Distance (front)

## TargetResponse

[TargetResponse](#) contains the (possibly area-summed or area-corrected) Area value when the associated TargetCompound row has its QuantByHeight column set to false. If this column is true, TargetResponse contains the same value as the Height column.

## UserCustomCalculation

[UserCustomCalculation](#) stores a result from a custom calculation.

UserCustomCalculation work with an undocumented scripting mechanism.

## UserCustomCalculation1

[UserCustomCalculation1](#) stores a result from a custom calculation.

UserCustomCalculation work with an undocumented scripting mechanism.

## UserCustomCalculation2

[UserCustomCalculation2](#) stores a result from a custom calculation.

UserCustomCalculation work with an undocumented scripting mechanism.

## UserCustomCalculation3

[UserCustomCalculation3](#) stores a result from a custom calculation.

UserCustomCalculation work with an undocumented scripting mechanism.

## UserCustomCalculation4

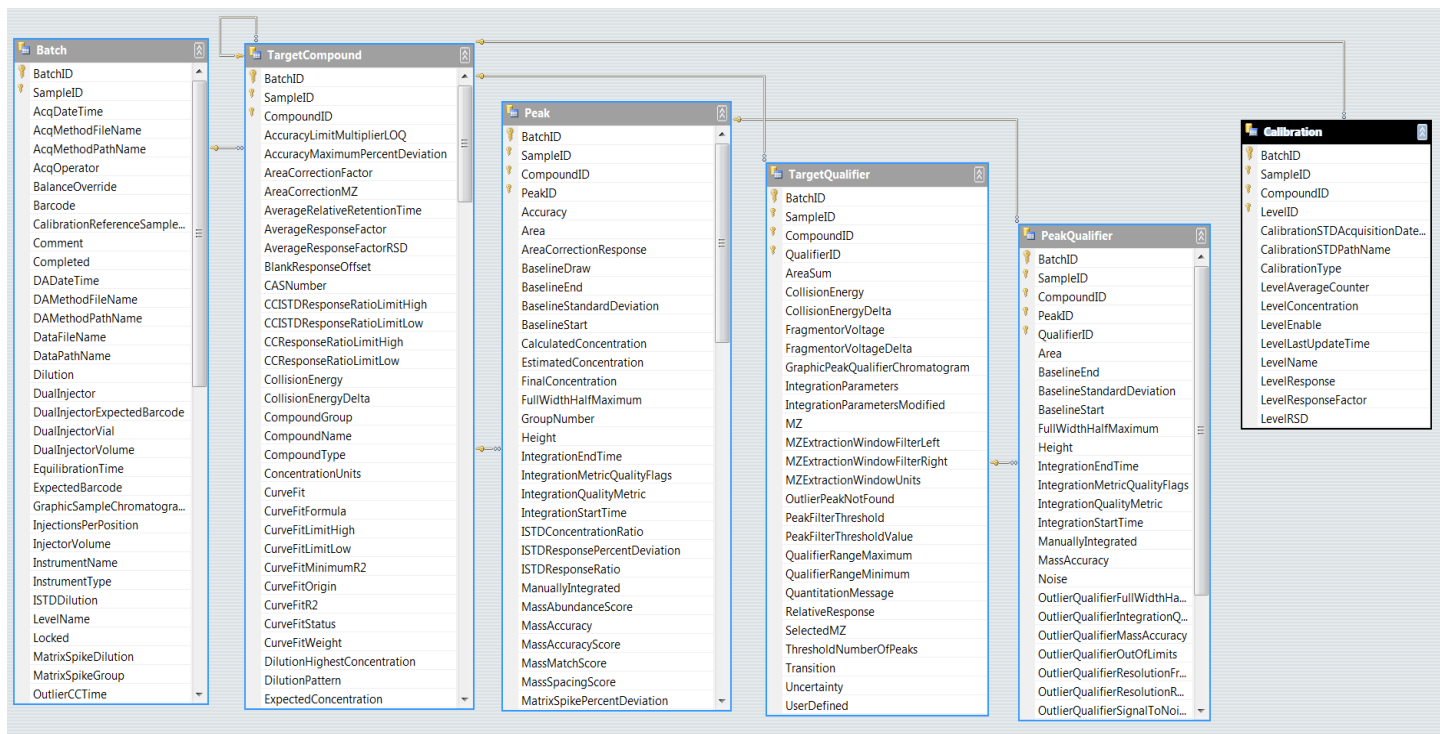
[UserCustomCalculation4](#) stores a result from a custom calculation.

UserCustomCalculation work with an undocumented scripting mechanism.

## Width

[Width](#) contains the integrator-determined peak width, in units of minutes, of the peak represented by this Peak row.

# Calibration Table



## Primary Key

{[BatchID](#), [SampleID](#), [CompoundID](#), [LevelID](#)} serves as the primary key. The composite of the [BatchID](#) and [SampleID](#) and [CompoundID](#) and [LevelID](#) and unique identify each row in this table. The keys in the Quantitation DataSet are not show in the user interface.

A primary key value must be unique with in the table. A composite key is a primary key that incorporates more than one column.

## BatchID

[BatchID](#) uniquely identifies the batch. [BatchID](#) is part of the composite primary key.

The [BatchID](#) is typically set to -1 because Batch-at-a-Glance analyzes one batch.

## SampleID

[SampleID](#) uniquely identifies the sample in the batch. [SampleID](#) is part of the composite primary key.

Thus, each sample in the batch is assigned a unique [SampleID](#).



## CompoundID

[CompoundID](#) uniquely identifies the sample in the batch. CompoundID is part of the composite primary key. Thus, each compound in the batch is assigned a unique CompoundID.

## LevelID

[LevelID](#) uniquely identifies the peak(s) for this compound. LevelID is part of the composite primary key.

Thus, each level in this calibration for this compound is assigned a unique LevelID.

## CalibrationSTDAcquisitionDateTime

[CalibrationSTDAcquisitionDateTime](#) records the date and time of the data file that is used to establish the calibration row.

## CalibrationSTDPathName

[CalibrationSTDPathName](#) names a persistent store of the data used to establish this calibration level. It's a full path name.

## CalibrationType

[CalibrationType](#) sub classifies or partitions the set of Calibration rows associated with a TargetCompound. CalibrationType designates the type of sample involved in the calibration curve. Is optional and not normally used.

One possible application is to partition six Levels into a five-point Daily Calibration and a one-point Continuing Calibration. The names DailyCalibration and ContinuingCalibration would be applied accordingly to these six levels.

Enum Name	UI Name	Xpath expression
Calibration	Calibration	*//CalibrationType[.='Calibration']
QC	QC	*//CalibrationType[.='QC']
Method	Method	*//CalibrationType[.='Method']
CC	CC	*//CalibrationType[.='CC']
ZeroStandard	Zero Standard	*//CalibrationType[.='ZeroStandard']

## LevelAverageCounter

[LevelAverageCounter](#) tallies the number of times the LevelResponse value for this Calibration row has been arithmetically averaged since the last time the LevelResponse value was completely replaced, or the inception of this Calibration row, whichever occurred later.

## LevelConcentration

[LevelConcentration](#) is the nominal concentration value for this calibration units. LevelConcentration is expressed in units as given by the ConcentrationUnits value in the associated TargetCompound row.

# LevelEnable

[LevelEnable](#) is true if and only if the (LevelConcentration, LevelResponse) point for this Calibration row is in play in terms of the calibration equation for the associated TargetCompound.

Method Table						
Time Segment: <All>		Compound: Cocaine-d3		Reset Table View		
Quantifier						
Name	TS	Scan	Type	Dil. High Conc.	Units	
Cocaine	1	MRM	Target	125.0000	ng/ml	
Calibration						
Level	Type	Conc.	Response	Enable	Cal. Path	
L1	Calibration	2.5000	5189	<input checked="" type="checkbox"/>	CMAMCal_L1.d	
L2	Calibration	5.0000	9716	<input type="checkbox"/>	CMAMCal_L2.d	
L2	QC	5.0000	9246	<input checked="" type="checkbox"/>	CMAMQC_L2.d	
L3	Calibration	12.5000	25187	<input checked="" type="checkbox"/>	CMAMCal_L3.d	
L4	Calibration	25.0000	50703	<input checked="" type="checkbox"/>	CMAMCal_L4.d	
L4	QC	25.0000	48582	<input checked="" type="checkbox"/>	CMAMQC_L4.d	
L5	Calibration	125.0000	199967	<input checked="" type="checkbox"/>	CMAMCal_L5.d	

For example, the sample acquired in CMAMCal\_L2.d has the compound Cocaine calibration point disabled.

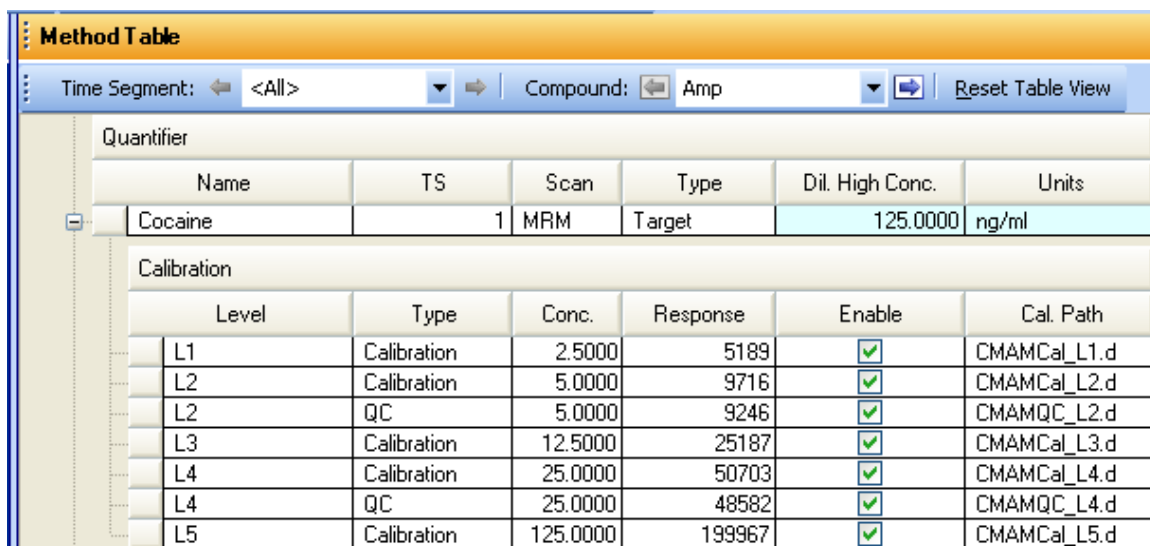
# LevelLastUpdateTime

[LevelLastUpdateTime](#) records the date and time for last change to the calibration row. This column is set whenever the calibration row is updated or analyzed.

# LevelName

[LevelName](#) is a descriptive string for this Calibration row.

LevelName connects a calibration or QC sample with a concentration and allows the association of replicate samples together.



Method Table					
Time Segment: <All>		Compound: Amp		Reset Table View	
Quantifier					
Name	TS	Scan	Type	Dil. High Conc.	Units
Cocaine	1	MRM	Target	125.0000	ng/ml
Calibration					
Level	Type	Conc.	Response	Enable	Cal. Path
L1	Calibration	2.5000	5189	<input checked="" type="checkbox"/>	CMAMCal_L1.d
L2	Calibration	5.0000	9716	<input checked="" type="checkbox"/>	CMAMCal_L2.d
L2	QC	5.0000	9246	<input checked="" type="checkbox"/>	CMAMQC_L2.d
L3	Calibration	12.5000	25187	<input checked="" type="checkbox"/>	CMAMCal_L3.d
L4	Calibration	25.0000	50703	<input checked="" type="checkbox"/>	CMAMCal_L4.d
L4	QC	25.0000	48582	<input checked="" type="checkbox"/>	CMAMQC_L4.d
L5	Calibration	125.0000	199967	<input checked="" type="checkbox"/>	CMAMCal_L5.d

For example, two samples one Calibration and one QC are run at level L2. All samples run at level L2 share the same concentration.

When multiple calibration samples are run at the same level, these calibration samples are considered replicates.

Note that a separate LevelName can denote a QC concentration, independent of the Calibration concentrations.

# LevelResponse

[LevelResponse](#) is the response value associated with this calibration level. LevelResponse can be height or area based on the QuantByHeight flag of the associated TargetCompound row.

# LevelResponseFactor

[LevelResponseFactor](#) is the Response / ISTDConcentration for ISTD corrected analysis. LevelResponseFactor is just the Response / Concentration.

# LevelRSD

[LevelRSD](#) is the relative standard deviation of the enabled calibration points (replicates) at a particular level.

This calibration level metric is computed as follows. For each calibration level  $n = 1 \dots N$ , the average, standard deviation of the current compound's [LevelResponse](#) are calculated over all enabled replicates ( $m=1 \dots M_n$ ) at calibration level  $n$ :

$$Avg_n = \frac{1}{M_n} \sum_{m=1}^{M_n} LevelResponse_{m,n}$$

$$SD_n = \sqrt{\frac{1}{M_n - 1} \sum_{m=1}^{M_n} (LevelResponse_{m,n} - Avg_n)^2}$$

For each calibration level  $n$  with  $M_n > 1$ , LevelRSD is set as follows:

$$LevelRSD_n = \frac{SD_n}{Avg_n} \times 100$$

where LevelRSD is %RSD or the relative standard deviation (RSD) of all enabled replicates in level  $n$ , expressed in percent. If only one replicate exists at a particular level  $M$ , LevelRSD is set to NULL.

# Outliers Overview

Outliers is a mechanism built into Batch-at-a-Glance that enables the identification of measurements that are outside set boundaries. The boundaries are set in the method and the measurements that are calculated as outliers (exceptions) are identified by assigning a flag {High, Low} to a specified Outlier column. In addition, the outlier is identified in the Batch-at-a-Glance user interface by marking the associated column.

## Outliers Enabled by Default

Several outliers are considered applicable enough to be enabled by default:

Outlier	Associated Column/Table	Comment
Integration Quality Metric	<a href="#">IntegrationMetricQualityFlags</a> (Peak table)	Defaulted: Using Agile Integrator
Qualifier Integration Quality Metric	<a href="#">IntegrationMetricQualityFlags</a> (PeakQualifier table)	Defaulted: Using Agile Integrator
Peak Not Found	OutlierPeakNotFound (Peak table)	
Qualifier Peak Not Found	OutlierPeakNotFound (PeakQualifier table)	
Accuracy	<a href="#">Accuracy</a>	Defaulted: +/-20%
Qualifier Ratio	<a href="#">QualifierResponseRatio</a> (PeakQualifier)	Defaulted: +/- 20%
RetentionTime	<a href="#">RetentionTime</a>	Defaulted: +/- 5% relative
Relative Retention Time	<a href="#">RetentionTime</a>	Defaulted: +/- 10% relative



## Summary of Outlier Specifications

Outlier Type	Outlier Flags	Highlighted Column	Sample Types	Column Type
Accuracy	Low, High	Peak.Accuracy	Calibration, QC, CC	All
Alternative Peak	Low, High	Peak.AlternativePeakRTDiff	All	All
Average Response Factor	Low	TargetCompound.AverageResponseFactor	All	All
Average Response Factor RSD	High	TargetCompound.AverageResponseFactorRSD	All	All
Blank Concentration	High	Peak.CalculatedConcentration	Blank	Tar
Blank Response	High	Peak.TargetResponse	Blank, DoubleBlank	Tar All Dou
CC Response Ratio	Low, High	Peak.TargetResponse	CC	Tar
CC ISTD Response Ratio	Low, High	Peak.TargetResponse	CC	ISTD
CC Average Response Factor	Low, High	TargetCompound.AverageResponseFactor	CC	All
CC Relative Response Factor	Low	Peak.TargetResponse	CC	Tar
CC Retention Time	Low, High	Peak.RetentionTime	CC	All
CC Time	High	Sample.AcqDateTime	All	N/A
Calibration Range	Low, High	Peak.CalculatedConcentration	All except blanks, Calibration, QC and CC	All
Capacity Factor	Low	Peak.CapacityFactor	All except blanks	All
Curve Fit R2	Low	TargetCompound.CurveFitR2	All	All
Custom Calculation	Low, High	TargetCompound.UserCustomCalculation	All	Tar
Full Width Half Maximum	Low, High	Peak.FullWidthHalfMaximum	All	All
Integration Quality Metric	Low, High	Peak.IntegrationQualityMetric	All	All
ISTD Response	Low, High	Peak.TargetResponse	All except DbIBlank	ISTD
ISTD Response Percent Deviation	Low, High	Peak.ISTDResponsePercentDeviation	All except DbIBlank	ISTD
Library Match Score	Low	Peak.ReferenceLibraryMatchScore	All	All
Limit of Detection	Low	Peak.CalculatedConcentration	All except blanks	All
Limit of Quantitation	Low	Peak.CalculatedConcentration	All except blanks	All
Mass Accuracy	Low, High	Peak.MassAccuracy	All	All
Mass Match Score	Low	Peak.MassMatchScore	All	All
Matrix Spike	Low, High	Peak.FinalConcentration	Matrix, MatrixDup	Ma
Matrix Spike Group Recovery	Low, High	Peak.MatrixSpikePercentRecovery	Matrix, MatrixDup	All
Matrix Spike Percent Recovery	Low, High	Peak.MatrixSpikePercentRecovery	Matrix, MatrixDup	Ma
Matrix Spike Percent	High	Peak.MatrixSpikePercentDeviation	Matrix, MatrixDup	Ma



Deviation				
Method Detection Limit	Low	Peak.CalculatedConcentration	All except blanks	All
Peak FWHM	Low, High	Peak.FullWidthHalfMaximum	All	All
Peak Not Found	Low	TargetCompound.TargetResponse	All except blanks	All Blanks
Peak Symmetry	Low, High	Peak.Symmetry	All	All
Qualifier Coelution Score	Low	PeakQualifier.CoelutionScore	All	All
Qualifier Integration Quality Metric	Low, High	PeakQualifier.IntegrationQualityMetric	All	All
Qualifier Peak Not Found	Low	TargetQualifier.QualifierResponseRatio	All except blanks	All Blanks
Qualifier Ratio	Low, High	PeakQualifier.QualifierResponseRatio	All except double blank	All
QC	Low, High	Peak.CalculatedConcentration	QC	Tar
QC RSD	High	Peak.TargetResponse	QC	Tar
QC LCS	Low, High	Peak.MatrixSpikePercentRecovery	QC (Info. column Contains LCSA or LCSB)	All
QValue	Low	Peak.QValueComputed	All	All
Relative Response Factor	Low, High	Peak.TargetResponse	All	All
Relative Retention Time	Low, High	Peak.RelativeRetentionTime	All	All
Resolution Front	Low	Peak.ResolutionFront	All	All
Resolution Rear	Low	Peak.ResolutionRear	All	All
Response Check	Low	Peak.TargetResponse	ResponseCheck	Tar
Response Factor	Low, High	Peak.TargetResponse	All	All
Retention Time	Low, High	Peak.RetentionTime	All	All
Sample Amount	Low, High	Peak.FinalConcentration	Sample	Tar
Sample RSD	High	Peak.SampleRSD	Sample	All
Saturation Recovery	High	Peak.SaturationRecoveryRatio	All	All
Signal To Noise Ratio	Low	Peak.SignalToNoiseRatio	All	All
Spectral Purity	Low	Peak.Purity	All except blanks	All
Surrogate	Low, High	Peak.FinalConcentration	All except blanks	Sur
Surrogate Percent Recovery	Low, High	Peak.SurrogatePercentRecovery	All except double blank	Sur

#### Notes:

A \* indicates that if the primary peak is not found, the compound and its containing sample will be flagged with a quantitation message, not with an outlier flag.

Throughout this table, "blanks" refers to all samples of type Blank and Double Blank.

Integration Quality Metric outlier is enabled only if a parameterless integrator (Agile integrator or MS-MS integrator) is used.

Qualifier Integration Quality Metric outlier is enabled only if a parameterless integrator (Agile integrator or MS-MS integrator) is used.

For the QC RSD outlier, all QC samples in a level will be flagged.

Relative Response Factor and Relative Retention Time outliers apply only to compounds that have an ISTD.

Response Factor outlier applies only to compounds that do NOT have an ISTD.

# Outliers

Below are detailed definitions and explanations of the outliers. Outliers are detected, calculated and reported during analysis. Outliers are useful in detecting results that exceed defined limits. These exceptions focus the analyst on the sample and compounds results that need review.

## Peak Result

This set of outliers are grouped together to handle exceptions related to Peak Results.

## Peak Not Found

This outlier metric is a measure of whether the compound's target ion has an associated peak. This outlier applies to all compound types and all sample types except Double blank and Blank, it also applies to ISTD compounds in Blank sample.

This outlier metric is determined by looking for the associated Peak row for that compound and determining if that peak row exists.-

The outlier is set to Low if the Peak row does not exist.

## Retention Time

This outlier metric is a measure of whether the current peak is within the Retention Time (RT) window. This outlier applies to the primary peak of all compound types and all sample types.

This outlier metric is determined by comparing the peak's retention time ([RetentionTime](#) in the Peak table) against the method's retention time ([RetentionTime](#) in the Target Compound table) and testing if the deviation is within the retention time window ([RetentionTimeWindow](#)), which can be expressed either in minutes or percent, as defined by [RetentionTimeWindowUnits](#). If [RetentionTimeWindowUnits](#) are Minutes, the outlier is set as follows:

$$\text{High if } RT > RT_{\text{method}} + \frac{1}{2} RT_{\text{Window}}$$

$$\text{Low if } RT < RT_{\text{method}} - \frac{1}{2} RT_{\text{Window}}$$

If [RetentionTimeWindowUnits](#) are Percent, the outlier is set as follows:

$$\text{High if } RT > RT_{method} \left( 1 + \frac{1}{2} \frac{RTWindow}{100} \right)$$

$$\text{Low if } RT < RT_{method} \left( 1 - \frac{1}{2} \frac{RTWindow}{100} \right)$$

When the outlier is set, the [RetentionTime](#) column of the Peak table is highlighted.

For the outlier to activate, the following columns must be set in the Quantitation Method Editor:

[RetentionTimeWindow](#)

[RetentionTimeWindowUnits](#)

## Relative Retention Time

This outlier metric is a measure of whether the current peak is within the Relative Retention Time (RRT) window. This outlier applies to the primary peak of all compound types except ISTD and all sample types.

This outlier metric is determined as follows:

For each enabled calibration point  $n = 1..N$  of a target compound's calibration table, compute  $RRT_n$  as the ratio of the calibration peak's retention time to the related ISTD retention time:

$$RRT_n = \frac{(RT_n)_{Compound}}{(RT_n)_{IS}}$$

Compute [AverageRelativeRetentionTime](#) ( $\overline{RRT}$ ) over  $N$  enabled Calibration and QC points:

$$\overline{RRT} = \frac{1}{N} \sum_{n=1}^N RRT_n$$

Compute the percent deviation of a peak's relative retention time (RRT):

$$RRTPercentDeviation = \frac{RRT - \overline{RRT}}{\overline{RRT}} \times 100$$

The outlier is set if the absolute value of the  $RRTPercentDeviation$  of a compound's peak is greater than [RelativeRetentionTimeMaximumPercentDeviation](#):

*High if  $RRT\text{PercentDeviation} > RRT\text{MaxPercentDeviation}$*

*Low if  $RRT\text{PercentDeviation} < -RRT\text{MaxPercentDeviation}$*

When the outlier is set, the [RelativeRetentionTime](#) column of the Peak table is highlighted.

For the outlier to activate, the following must be set in the Quantitation Method Editor:

Target must have a related ISTD

[RelativeRetentionTimeMaximumPercentDeviation](#)

**Example:**

[RelativeRetentionTimeMaximumPercentDeviation](#) = 5%.

Target's RetentionTime = 2.22 min.

ISTD's RetentionTime = 2.00 min.

[RelativeRetentionTime](#) =  $2.22 / 2.00 = 1.11$

[AverageRelativeRetentionTime](#) =  $\text{Sum}(RRT) / N$  for all the compound's enabled Calibration and QC points = 1.00

$RRT\text{PercentDeviation} = (1.11 - 1.00 / 1.00) * 100 = 11.1\%$

[RelativeRetentionTimeMaximumPercentDeviation](#) = 10%

Since the peak's [RelativeRetentionTimePercentDeviation](#) exceeds the [RelativeRetentionTimeMaximumPercentDeviation](#), this outlier is set to *High*.

## Integration Quality Metric

This outlier metric is a measure of the quality of the current peak's integration. This outlier applies to the primary peak of all compound types and all sample types.

This outlier metric is determined by examining the parameterless (MS-MS or Agile) integrator metric stored in the [IntegrationQualityMetric](#). If the peak's [IntegrationQualityMetric](#) is "Rejected" or "Inspect", the outlier is set to *High* and *Low*, respectively.

The integrated peak's [IntegrationQualityMetric](#) column is highlighted, and the outlier message describes the reason why the peak has been rejected or "inspect", as reported by the integrator in the [IntegrationMetricQualityFlags](#) column.

For the outlier to activate, the Integrator must be set to a parameterless (MS-MS or Agile) integrator.

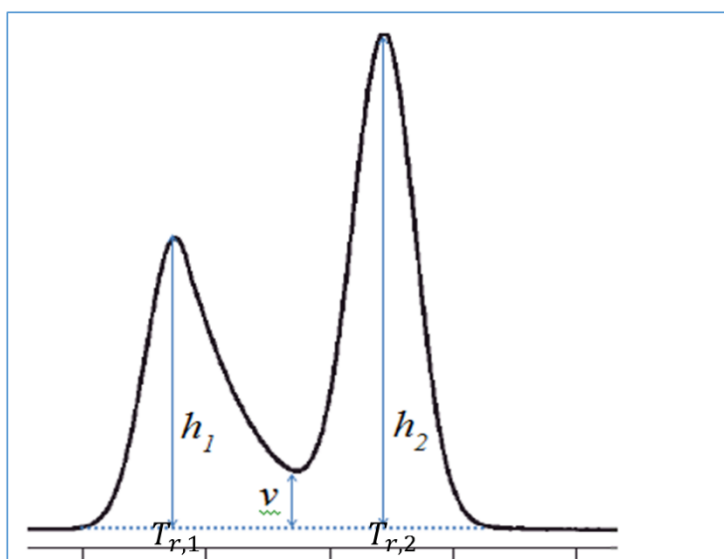
## Resolution

This outlier metric is a measure of how well two neighboring peaks are separated. This outlier applies to the primary peaks of all compound types and all sample types.

This outlier metric is determined by comparing the calculated resolution value of the primary peak against a user-defined limit [ResolutionLimit](#).

The outlier is set to *Low* or *High* based on different calculations

Peak resolution is calculated differently if different pharmacopeia is selected.



Pharmacopeia	Formula	Outlier
Default	$100 \times \left(1 - \frac{2v}{h_1 + h_2}\right)$	Low
USP	$2 \times (T_{r,2} - T_{r,1}) / (W_{b,1} + W_{b,2})$	Low
EU	$1.18 \times (T_{r,2} - T_{r,1}) / (W_{50,1} + W_{50,2})$	Low
JP	$1.18 \times (T_{r,2} - T_{r,1}) / (W_{50,1} + W_{50,2})$	Low
Valley Height/Peak Height	$100 \times v/h$	High
Valley Height/Peak Height Average	$100 \times \frac{2v}{h_1 + h_2}$	High
Valley Height/Peak Height Sum	$100 \times \frac{v}{h_1 + h_2}$	High

- $T_{r,2}$  is the retention time of the right peak in the peak pair.
- $T_{r,1}$  is the retention time of the left peak in the peak pair.
- $W_b$  is the peak width determined by the tangent method.
- $W_{50}$  is the peak width at 50% of the height of the peak.
- $h$  is the primary peak height
- $v$  is valley height, when it's calculated, a 3-point median filter is applied to the lowest point between the two peaks to handle the noisy signals

When the outlier is set, the [ResolutionFront and/or ResolutionRear](#) columns are highlighted.

For the outlier to activate, the following columns must be set in the Quantitation Method Editor:

- [ResolutionLimit](#)

## Symmetry

This outlier metric is a measure of whether the peak symmetry is below or above the preset limits. This outlier applies to the primary peaks of all compound types and all sample types.

This outlier metric is determined by comparing the calculated [Symmetry](#) value of the primary peak against a user-defined limits [SymmetryLimitLow](#) and [SymmetryLimitHigh](#)

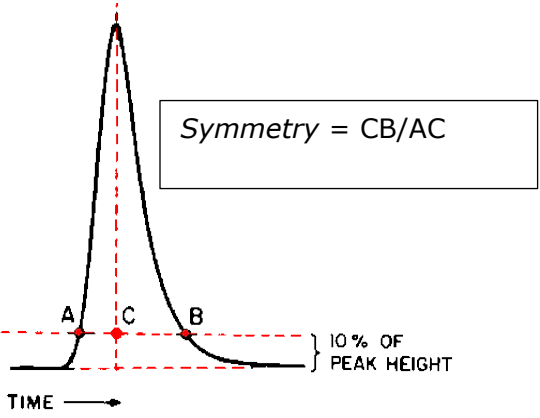
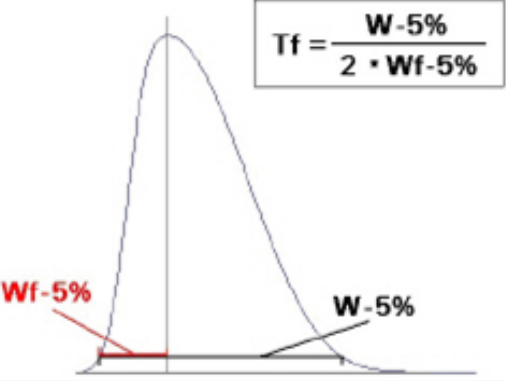
The outlier is set to *High* if

$Symmetry > SymmetryLimitHigh$

The outlier is set to *Low* if

$Symmetry < SymmetryLimitLow$

Peak symmetry is calculated as the ratio (at the 10% of the peak height) of the distance between the peak apex and the back side of the chromatographic curve to the distance between the peak apex and the front side of the chromatographic curve for default setting; and is calculated as the ratio (at the 5% of the peak height) of the peak width to the distance between the peak apex and the front side of the chromatographic curve for all other pharmacopeia settings.

Pharmacopeia	Formula
Default	 <p><math>Symmetry = CB/AC</math></p>
USP/EU/JP/CP	 <p><math>Tf = \frac{W-5\%}{2 \cdot Wf-5\%}</math></p>

When the outlier is set, the [Symmetry](#) column is highlighted.

For the outlier to activate, the following columns must be set in the Quantitation Method Editor:

- [SymmetryLimitHigh](#)
- [SymmetryLimitLow](#)



## Full Width Half Maximum

This outlier metric is a measure of whether the full width half maximum (FWHM) is outside the preset limit. This outlier applies to the primary peaks of all compound types and all sample types.

This outlier metric is determined by comparing the calculated [FullWidthHalfMaximum](#) value of the primary peak against a user-defined limits [FullWidthHalfMaximumLimitLow](#) and [FullWidthHalfMaximumLimitHigh](#).

The outlier is set to *High* if

$$\text{FullWidthHalfMaximum} > \text{FullWidthHalfMaximumLimitHigh}$$

The outlier is set to *Low* if

$$\text{FullWidthHalfMaximum} < \text{FullWidthHalfMaximumLimitLow}$$

Full width half maximum is calculated as the peak width at the half height.

When the outlier is set, the [FullWidthHalfMaximum](#) column is highlighted.

For the outlier to activate, the following columns must be set in the Quantitation Method Editor:

- [FullWidthHalfMaximumLimitHigh](#)
- [FullWidthHalfMaximumLimitLow](#)

## Purity

This outlier metric is a measure of whether the spectral purity of a peak is below the preset limit. This outlier applies to the primary peaks of all compound types except ISTD and all sample types except Blank and Double Blank.

This outlier metric is determined by comparing the calculated spectral purity of the primary peak, in percent, contained in the [Purity](#) column, against a user-defined minimum limit [MinimumPercentPurity](#). The outlier is set to *Low* if

$$Purity < MinimumPercentPurity$$

The purity calculation entails running a deconvolution on the entire chromatographic range of the sample. However, the new algorithm differs from the previously released versions (prior to B.05.02) in several important aspects:

- 1) The identification of the component that matches the target compound (the "target component") uses a different set of criteria that makes it more robust:
  - a. For each component found by deconvolution, the system finds all component spectrum peaks that fall within the m/z delta range of the target quantifier m/z.
  - b. For every such component spectrum peak, the system checks if the corresponding ion peak (EIC peak) has an apex within the RT range of the target quantifier peak.
  - c. The component with the largest such peak is identified as the target component.
- 2) If the system fails to find a target component for any given target compound, it re-tries by running the full-sample deconvolution in "high-resolution" mode, using a window size factor that is reduced by a factor of 2. The high-resolution results are cached and are searched for any target compound that cannot be found in the normal-resolution component list. The automatic generation of the high-resolution results allows many target components to be identified that were previously missed.
- 3) The system attempts to detect "double components" that share the same RT and base peak m/z. The presence of such component doublets can strongly bias the purity estimate to the downside. Component doublets can occur if the RT window size factor is too small. Therefore, the system attempts to recover automatically by re-running the full-sample deconvolution in "low-resolution" mode, using a window size factor that is increased by a factor of 2. The low-resolution results are cached and are searched for any target that is matched to a component doublet.
- 4) The new purity calculation uses a different formula that gives more meaningful results in cases of severe interference. (The old purity definition can yield zero purity for such cases.) The new definition of purity uses the following formula:

$$Purity(\text{Target compound}) = \text{Area}(\text{Target component shape}) / \text{SUM}(\text{Area}(\text{Contributing component shape}))$$

The SUM is over all contributing components. A contributing component is any component that has spectral peaks within m/z delta range of the target quantifier m/z and overlaps the target peak in retention time.

When the outlier is set, the [Purity](#) column is highlighted.

For the outlier to activate, the following columns must be set in the Quantitation Method Editor:

- [MinimumPercentPurity](#)
- [SpectrumExtractionOverride](#) set to "Deconvoluted Scan"

## Plates

This outlier metric is a measure of the column efficiency. A capillary column/any chromatography column does not contain anything resembling physical distillation plates or other similar features. Theoretical plate numbers are indirect measure of peak width for a peak at a specific retention time. Columns with plate numbers are considered to be more efficient than columns with lower plate numbers. A column with a high number of plates will have a narrower peak at a given retention time than a column with a lower number of plates.

Different pharmacopeia uses different formulas to determine the value for Plates.

Pharmacopeia	Formula
USP / CP	$16 * (Tr / Wb) ^2$
EU / JP / CP	$5.54 * (Tr / W50) ^2$

- Tr is the retention time
- Wb is the peak width determine by the tangent method.
- W50 is the peak width at 50% of the height of the peak.

This outlier metric is determined by comparing the calculated plate numbers of the primary peak ([Plates](#) in the Peak table) against a user-defined minimum limit ([PlatesLimit](#)). The outlier is set to *Low* if

$$Plates < PlatesLimit$$

When the outlier is set, the [Plates](#) column is highlighted.

For the outlier to activate, the following columns must be set in the Quantitation Method Editor:

[PlatesLimit](#)

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Chinese Pharmacopoeia allows either choice of calculation.

## Capacity Factor

This outlier metric is a measure of the retention of an analyte on the chromatographic column. It is the ratio of the amount of time a solute spends in the stationary and mobile phases. For example, a solute with a  $k' = 6$  is twice as retained by the stationary phase (but not the column) as a solute with a  $k' = 3$ . The retention factor does not provide absolute retention information; it provides relative retention information. An unretained compound has a retention factor of 0.

$$k' = (T_r - T_0) / T_0$$

where  $T_r$  is the retention time of the analyte.  $T_0$  is the retention time of an unretained compound, i.e., column void time ([ColumnVoidTime](#)). The outlier is set to Low if

$$\text{CapacityFactor} < \text{CapacityFactorLimit}$$

When the outlier is set, the [CapacityFactor](#) column is highlighted.

For the outlier to activate, the following column must be set in the Quantitation Method Editor:

[CapacityFactorLimit](#)

## Signal To Noise Ratio

This outlier metric is a measure of whether the peak signal-to-noise ratio is below the preset limit. This outlier applies to the primary peaks and qualifiers of all compound types and all sample types.

This outlier metric is determined by comparing the calculated signal-to-noise ratio of the primary peak ([SignalToNoiseRatio](#) in the Peak table) against a user-defined minimum limit ([MinimumSignalToNoiseRatio](#)). The outlier is set to *Low* if

$$\text{SignalToNoiseRatio} < \text{MinimumSignalToNoiseRatio}$$

When the outlier is set, the [SignalToNoiseRatio](#) column is highlighted.

For the outlier to activate, the following columns must be set in the Quantitation Method Editor:

[MinimumSignalToNoiseRatio](#)

## Limit Of Detection

This outlier metric is a measure of whether the current quantitated amount is below the limit of detection (LOD) threshold. This outlier applies to the primary peaks of all compound types and all sample types except:

- Blank

- Double Blank

If no primary peak is found, the sample is flagged with a quantitation error message, not with an outlier flag.

This outlier metric is determined by comparing the quantitated amount ([CalculatedConcentration](#)) against a user-defined limit of detection ([LimitOfDetection](#)). The outlier is set to *Low* if

$$\text{CalculatedConcentration} < \text{LimitOfDetection}$$

When the outlier is set, the [CalculatedConcentration](#) column is highlighted.

For the outlier to activate, the following columns must be set in the Quantitation Method Editor:  
[LimitOfDetection](#)

## Limit Of Quantitation

This outlier metric is a measure of whether the current quantitated amount is below the limit of quantitation (LOQ) threshold. This outlier applies to the primary peaks of all compound types and all sample types except Blank and Double Blank. If no primary peak is found, the sample is flagged with a quantitation error message, not with an outlier flag.

This outlier metric is determined by comparing the quantitated amount ([CalculatedConcentration](#)) against a user-defined limit of quantitation ([LimitOfQuantitation](#)). The outlier is set to *Low* if

$$\text{CalculatedConcentration} < \text{LimitOfQuantitation}$$

When the outlier is set, the [CalculatedConcentration](#) column is highlighted.

For the outlier to activate, the following columns must be set in the Quantitation Method Editor:

[LimitOfQuantitation](#)

## Method Detection Limit

This outlier metric is a measure of whether the current quantitated amount is below the method detection limit (MDL) threshold. This outlier applies to the primary peaks of all compound types and all sample types except Blank and Double Blank. If no primary peak is found, the sample is flagged with a quantitation error message, not with an outlier flag.

This outlier metric is determined by comparing the quantitated amount ([CalculatedConcentration](#)) against a user-defined method detection limit ([MethodDetectionLimit](#)). The outlier is set to *Low* if

$$\text{CalculatedConcentration} < \text{MethodDetectionLimit}$$

When the outlier is set, the [CalculatedConcentration](#) column is highlighted.

For the outlier to activate, the following columns must be set in the Quantitation Method Editor:  
[MethodDetectionLimit](#)

## Qualifier

This set of outliers are grouped together to handle exceptions related to Qualifiers.

## Qualifier Peak Not Found

This outlier metric is a measure of whether the compound's qualifier ions have associated peaks. This outlier applies to all compound types and all sample types except Double blank and Blank, it also applies to ISTD compounds in Blank sample.

This outlier metric is determined by looking for the associated PeakQualifier row for that compound and determining if that peak row exists.

The outlier is set to Low if the PeakQualifier row does not exist when target ion is found.

## Qualifier QValue

This outlier metric is a measure of the fidelity of the observed qualifier ratios versus the nominal qualifier ratios. The QVALUE function is a well-defined statistic that yields an efficient measure of the "goodness of fit" of the observed qualifier ratios to the nominal qualifier ratios.

For all hits a QVALUE is computed as described here. For Target Compound Entries with no qualifier signals, the QVALUE is defined as 100. For Target Compound Entries with k qualifier signals  $q_i$ ,  $1 \leq i \leq k$ , define  $r_i$  as the expected ratio of qualifier peak for  $q_i$  to the target peak. Then define  $r_i'$  as the observed qualifier ratio as determined by the above Qualifier Ratio Computation. Now define the total ratio deviation D:

$$D = \frac{\sum_{1 \leq i \leq k} (100|r_i - r_i'|)(\ln(100r_i + 1))^2}{21.3 \sum_{1 \leq i \leq k} r_i}$$

Then the QVALUE is the closest integer to  $\max \{ 100 - D, 1 \}$ .

This outlier metric is determined by comparing the [QValueComputed](#) of the qualifier ion against a user defined limit [QValueMinimum](#).

The outlier is set to *Low* if

$$QValueComputed < QValueMinimum$$

When the outlier is set, the [QValueComputed](#) column is highlighted.

For the outlier to activate, the following columns must be set in the Quantitation Method Editor:

- [QValueMinimum](#)

## Qualifier Ratio

This outlier metric is a measure of whether the current qualifier's peak ratio is above or below the qualifier peak ratio limits. In preparing a quantitation method, you can assign a ratio to the quantifier and qualifier ions with an associated uncertainty. This criterion is useful in confirming



the identity of the compound analyzed because that compound follows a certain fragmentation pattern which results in the predicted ratios. This outlier applies to all compounds and all sample types except Double Blank.

This outlier metric is determined by comparing the response (area or height) of the qualifier signal to the response of the quantifier signal. The response ratio, stored as [QualifierResponseRatio](#), is tested against [QualifierRangeMaximum](#) and [QualifierRangeMinimum](#). These limits are computed as follows:

If [UncertaintyRelativeOrAbsolute](#) = Absolute,

$$\text{QualifierRangeMinimum} = \text{RelativeResponse} - \text{Uncertainty}$$

$$\text{QualifierRangeMaximum} = \text{RelativeResponse} + \text{Uncertainty}$$

If [UncertaintyRelativeOrAbsolute](#) = Relative,

$$\text{QualifierRangeMinimum} = \text{RelativeResponse} \times (100 - \text{Uncertainty})/100$$

$$\text{QualifierRangeMaximum} = \text{RelativeResponse} \times (100 + \text{Uncertainty})/100$$

The outlier is set to *High* if

$$\text{QualifierResponseRatio} > \text{QualifierRangeMaximum}$$

The outlier is set to *Low* if

$$\text{QualifierResponseRatio} < \text{QualifierRangeMinimum}$$

When the outlier is set, the [QualifierResponseRatio](#) column is highlighted.

For the outlier to activate, the following must be set in the Quantitation Method Editor:

[Uncertainty \(percent\)](#)

[UncertaintyRelativeOrAbsolute](#)

### Example:

For a qualifier ion that has a [QualifierResponseRatio](#) of 40% and a % uncertainty of 20: If [UncertaintyRelativeOrAbsolute](#) is set to "Relative", the acceptable range is from

$\text{QualifierRangeMinimum} = 32\%$  to

*QualifierRangeMaximum* =48%.

If UncertaintyRelativeOrAbsolute is set to "Absolute", the acceptable range is from

*QualifierRangeMinimum* =20% to

*QualifierRangeMaximum* =60%.

## Qualifier Coelution Score

This outlier metric is a measure of how well this qualifier ion coelutes with the quantifier ion. The Coelution score uses the retention time of the quantifier ion and the quantifier ion as well as the peak width and the peak symmetry of the quantifier ion and the qualifier ion.

This outlier metric is determined by comparing the calculated CoelutionScore value of the qualifier ion against a user-defined limits CoelutionScoreLimit.

The outlier is set to *Low* if

$$CoelutionScore < CoelutionScoreLimit$$

When the outlier is set, the CoelutionScore column is highlighted.

For the outlier to activate, the following columns must be set in the Quantitation Method Editor:

- CoelutionScoreLimit

## Qualifier Integration Quality Metric

This outlier metric is a measure of the quality of a qualifier peak's integration. This outlier applies to all the qualifier peaks of all compounds and sample types.

This outlier metric is determined by examining the parameterless (MS-MS or Agile) integrator metric stored in the IntegrationQualityMetric of the PeakQualifier table. If the peak's IntegrationQualityMetric is "Rejected" or "Inspect", the outlier is set to *High* and *Low*, respectively. The integrated peak's IntegrationQualityMetric column is highlighted, and the outlier message describes the reason why the peak has been rejected or "inspect", as reported by the MS-MS integrator in the IntegrationMetricQualityFlags column.

When the outlier is set, the IntegrationQualityMetric column of the PeakQualifier table is highlighted.

For the outlier to activate, the Integrator must be set to MS-MS or Agile integrator.

## Qualifier Peak Symmetry

This outlier metric is a measure of whether the qualifier peak symmetry is below or above the preset limits. This outlier applies to the qualifier peaks of all compound types and all sample types.

This outlier metric is determined by comparing the calculated [Symmetry](#) value of the primary peak against a user-defined limits [SymmetryLimitLow](#) and [SymmetryLimitHigh](#)

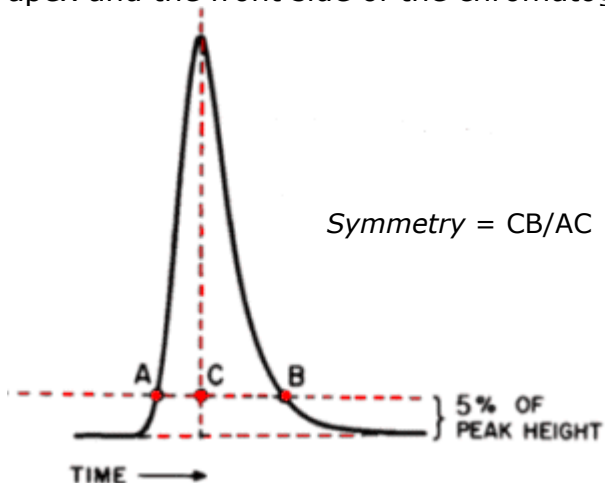
The outlier is set to *High* if

$$\text{Symmetry} > \text{SymmetryLimitHigh}$$

The outlier is set to *Low* if

$$\text{Symmetry} < \text{SymmetryLimitLow}$$

Peak symmetry is calculated as the ratio (at the 5% of the peak height) of the distance between the peak apex and the back side of the chromatographic curve to the distance between the peak apex and the front side of the chromatographic curve.



When the outlier is set, the [Symmetry](#) column is highlighted.

For the outlier to activate, the following columns must be set in the Quantitation Method Editor:

- [SymmetryLimitHigh](#)
- [SymmetryLimitLow](#)

## Qualifier Peak Full Width Half Maximum

This outlier metric is a measure of whether the full width half maximum (FWHM) of a qualifier peak is outside the preset limit. This outlier applies to all qualifier peaks of all compound types and all sample types.

This outlier metric is determined by comparing the calculated [FullWidthHalfMaximum](#) value of the qualifier peak against a user-defined limits [FullWidthHalfMaximumLimitLow](#) and [FullWidthHalfMaximumLimitHigh](#).

The outlier is set to *High* if

$$FullWidthHalfMaximum > FullWidthHalfMaximumLimitHigh$$

The outlier is set to *Low* if

$$FullWidthHalfMaximum < FullWidthHalfMaximumLimitLow$$

Full width half maximum is calculated as the peak width at the half height.

When the outlier is set, the [FullWidthHalfMaximum](#) column is highlighted.

For the outlier to activate, the following columns must be set in the Quantitation Method Editor:

- [FullWidthHalfMaximumLimitHigh](#)
- [FullWidthHalfMaximumLimitLow](#)

## Number Of Verified Ions

This outlier metric is a measure of whether the number of verified ions is outside the predefined limit. This outlier applies to all compound types and all sample types.

This outlier metric is determined by comparing the calculated [NumberOfVerifiedIons](#) value of the against a user-defined limits [NumberOfVerifiedIonsLimit](#)

The outlier is set to *Low* if

$$NumberOfVerifiedIons < NumberOfVerifiedIonsLimit$$

Number of verified ions is the number of ions (including quantifier and qualifiers defined in method) that meet the SANTE guideline criteria, when the [VerifiedIonType](#) is SANTE\_AccurateMass or null, it include S/N, coelution score, and mass accuracy. Number of verified ions is calculated based on the S/N, coelution score, and mass accuracy outliers. Only if an ion doesn't have any of the above outliers, this ion is verified. When the [VerifiedIonType](#) is SANTE\_UnitMass, it includes qualifier ratio, S/N, and coelution score, Only if an ion doesn't have any of the above outliers, this ion is verified.

# ISTD

This set of outliers are grouped together to handle exceptions related to internal standard correction (ISTD).

## ISTD Response

This outlier metric is a measure of whether the internal standard response (area or height) is above or below preset limits. This outlier applies to the primary peak of every ISTD compound in all sample types except Double Blank. If no primary peak is found, the sample is flagged with a quantitation error message, not with an outlier flag.

This outlier metric is determined by comparing the [TargetResponse](#) column of the primary peak of an ISTD compound against the limits [ISTDResponseLimitLow](#), [ISTDResponseLimitHigh](#).

The outlier is set to *High* if

$$\textit{TargetResponse} > \textit{ISTDResponseLimitHigh}$$

The outlier is set to *Low* if

$$\textit{TargetResponse} < \textit{ISTDResponseLimitLow}$$

When the outlier is set, the [TargetResponse](#) column is highlighted.

For the outlier to activate, the following columns must be set in the Quantitation Method Editor:

- [ISTDResponseLimitLow](#)
- [ISTDResponseLimitHigh](#)

## ISTD Response Percent Deviation

This outlier metric is a measure of whether the internal standard response (area or height) deviates more than the user defined percent limits from the average ISTD response calculated from the existing calibration.

A poor injection as well as matrix enhancement or suppression could cause the ISTD response to exceed the limits.

This outlier applies to the primary peak of every ISTD compound in all sample types except Double Blank. If no primary peak is found, the sample is flagged with a quantitation error message, not with an outlier flag.

The outlier is set to *High* if

$$\textit{ISTDResponsePercentDeviation} > \textit{ISTDReponseMaximumPercentDeviation}$$

Where

$$ISTDResponsePercentDeviation = \frac{ISTDResponse_i - Average(ISTDResponse)_{calibration}}{Average(ISTDResponse)_{calibration}} \times 100$$

The outlier is set to *Low* if

$$ISTDResponsePercentDeviation < ISTDReponseMinimumPercentDeviation)$$

To support backward compatibility, if only a maximum limit is set, the lower limit will be set to  $-ISTDReponseMinimumPercentDeviation$ .

When the outlier is set, the [ISTDResponsePercentDeviation](#) column is highlighted.

For the outlier to activate, the following column must be set in the Quantitation Method Editor:

- [ISTDResponseMaximumPercentDeviation \(can set maximum limit only\)](#)
- [ISTDResponseMinimumPercentDeviation](#)

# Sample

This set of outliers are grouped together to handle exceptions related to Samples.

## Sample Amount

This outlier metric is a measure of whether the current quantitated amount is above or below preset sample limits. This outlier applies to the primary peak of every Target compound in all samples of type Sample. If no primary peak is found, the sample is flagged with a quantitation error message, not with an outlier flag.

This outlier metric is determined by comparing the quantitated amount adjusted by the [Multiplier \(FinalConcentration\)](#) against the limits [SampleAmountLimitLow](#), [SampleAmountLimitHigh](#).

The outlier is set to *High* if

$$FinalConcentration > SampleAmountLimitHigh$$

The outlier is set to *Low* if

$$FinalConcentration < SampleAmountLimitLow$$

When the outlier is set, the [FinalConcentration](#) column is highlighted.

For the outlier to activate, the following columns must be set in the Quantitation Method Editor:

[SampleAmountLimitLow](#)

[SampleAmountLimitHigh](#).

## Sample Relative Standard Deviation

This outlier metric is a measure of whether the standard deviation of the final concentration for samples within the same [SampleGroup](#) is greater than a pre-determined limit. For samples that are not assigned any [SampleGroup](#), they are considered to be in the same [SampleGroup](#). This outlier applies to the primary peak of every Target compound in all samples of type Sample. If no primary peak is found, the sample is flagged with a quantitation error message, not with an outlier flag.

This outlier is calculated as follows:

For each SampleGroup  $x$ , calculate the average and standard deviation of current compound's FinalConcentration over all Sample samples ( $m=1...M_x$ )

$$Avg_x = \frac{1}{M_x} \sum_{m=1}^{M_x} FinalConcentration_{m,x}$$



$$SD_x = \sqrt{\frac{1}{M_x - 1} \sum_{m=1}^{M_x} (FinalConcentration_{m,x} - Avg_x)^2}$$

$$\%RSD_x = \frac{SD_x}{Avg_x} \times 100$$

For each sample group, the outlier is set to *High* if

$$\%RSD_x > SampleMaximumPercentRSD$$

When the outlier is set, the [SampleRSD](#) column is highlighted.

For the outlier to activate, the following columns must be set in the Quantitation Method Editor:

[SampleMaximumPercentRSD](#)

## Blank

This set of outliers are grouped together to handle exceptions related to Blanks.

### Blank Concentration

This outlier metric is a measure of whether the calculated concentration for a compound in a blank sample is greater than the preset maximum limit. This outlier applies to the primary peaks of all Target compounds in all samples of type Blank.

This outlier metric is determined by comparing the quantitated amount ([CalculatedConcentration](#)) for each compound in a blank sample against that compound's user-defined maximum limit ([MaximumBlankConcentration](#)). The outlier is set to *High* if

$$CalculatedConcentration > MaximimBlankConcentration$$

When the outlier is set, the [CalculatedConcentration](#) column is highlighted.

For the outlier to activate, the following columns must be set in the Quantitation Method Editor:

[MaximumBlankConcentration](#)

## Blank Response

This outlier metric is a measure of whether the target response for a compound in a blank sample is greater than the preset maximum limit. This outlier applies to the primary peaks of all Target compounds in all samples of type Blank and DoubleBlank. This outlier also applies to all compounds in samples of type DoubleBlank.

This outlier metric is determined by comparing the target response for each compound in a blank sample against that compound's user-defined maximum limit ([MaximumBlankResponse](#)). The outlier is set to *High* if

$$\text{TargetResponse} > \text{MaximumBlankResponse}$$

When the outlier is set, the TargetResponse column is highlighted.

For the outlier to activate, the following columns must be set in the Quantitation Method Editor:  
[MaximumBlankResponse](#)

## Calibration

This set of outliers are grouped together to handle exceptions related to Calibration.

## Accuracy

This outlier metric is a measure of whether the quantitated amount for a calibration sample or QC or CC is above or below a pre-determined relative deviation from an expected value. This outlier applies to the primary peak of every compound type except ISTD in the Calibration, QC and CC samples. If no primary peak is found, the sample is flagged with a quantitation error message, not with an outlier flag.

This outlier metric is determined by examining the ratio of the peak's quantitated amount ([CalculatedConcentration](#)) to the expected amount ([ExpectedConcentration](#)). The Accuracy of quantitation of a given compound is defined as follows:

$$\text{Accuracy} = \frac{\text{CalculatedConcentration}}{\text{ExpectedConcentration}} \times 100$$

The Accuracy outlier is set to *Low* if

$$\text{Accuracy} < 100 - \text{MaxAccuracyDeviation}$$

The Accuracy outlier is set to *High* if

$$Accuracy > 100 + MaxAccuracyDeviation$$

For all but the lowest calibration level (the LOQ level), *MaxAccuracyDeviation* = [AccuracyMaximumPercentDeviation](#). For the lowest calibration level, *MaxAccuracyDeviation* is computed as follows:

$$\begin{aligned} MaxAccuracyDeviation (lowest\ calibration\ level) = \\ AccuracyMaximumPercentDeviation \\ \times AccuracyLimitMultiplierLOQ \end{aligned}$$

By default, [AccuracyLimitMultiplierLOQ](#) is set to 1. When the outlier is set, the [Accuracy](#) column is highlighted.

For the outlier to activate, the following columns must be set:

[AccuracyMaximumPercentDeviation](#)

[ExpectedConcentration](#)

[AccuracyLimitMultiplierLOQ](#)

## Average Response Factor

This outlier metric is a measure of whether the current compound has a calibration curve that satisfies the average response factor criteria. An average response factor flagged below the limit can indicate a poor response for the compound. This outlier applies to all compound types except ISTD and to all sample types.

This outlier metric is determined as follows:

For each enabled calibration point  $n=1\dots N$  in the compound's calibration table with a non-zero concentration, the system computes the LevelResponseFactor which is either the response factor (RF) or the relative response factor (RRF) of the calibration level, depending on whether the compound has an ISTD:

$$LevelResponseFactor_n = \begin{cases} RF_n, & \text{if no ISTD} \\ RRF_n, & \text{if ISTD} \end{cases}$$

$$RF_n = \frac{(LevelResponse)_n}{(LevelConcentration)_n}$$

$$RRF_n = \frac{LevelResponse_n \times ISTDConc_n}{LevelConc_n \times ISTDResponse_n}$$

Compute AverageResponseFactor over all enabled calibration points:

$$AverageResponseFactor = \frac{1}{N} \sum_{n=1}^N LevelResponseFactor_n$$

The outlier is set to *Low* if

$$AverageResponseFactor < MinimumAverageResponseFactor$$

When the outlier is set, the AverageResponseFactor column is highlighted.

For the outlier to activate, the following columns must be set in the Quantitation Method Editor:

MinimumAverageResponseFactor

Note that the value of MinimumAverageResponseFactor must be set knowing whether the compound has an ISTD or not.

## Average Response Factor RSD

This outlier metric is a measure of whether the standard deviation of response factor across the entire calibration curve is greater than a pre-determined limit. A response factor RSD flagged above the limit can indicate a poor calibration for the compound. This outlier applies to all compound types except ISTD and to all sample types.

This outlier metric is determined as follows:

Compute [AverageResponseFactor](#) over all enabled calibration points:

$$AverageResponseFactor = \frac{1}{N} \sum_{n=1}^N LevelResponseFactor_n$$

$$\sigma = \sqrt{\frac{\sum_{n=1}^N (LevelResponseFactor_n - AverageResponseFactor)^2}{N - 1}}$$

$$\%RSD = 100 \times \frac{\sigma}{AverageResponseFactor}$$

The outlier is set to *High* if

$$\%RSD > MaximumResponseFactorRSD$$

When the outlier is set, the [AverageResponseFactorRSD](#) column is highlighted.

For the outlier to activate, the following columns must be set in the Quantitation Method Editor:

[MaximumAverageResponseFactorRSD](#)

Note that the value of [MaximumAverageResponseFactorRSD](#) must be set knowing whether the compound has an ISTD or not.

## Calibration Range

This outlier metric is a measure of whether the current quantitated amount for non-calibration or non-QC samples is within the range of points comprising the calibration curve.

Note that Quality Controls (QCs) are not considered part of the calibration curve. This outlier applies to the primary peak of target compound only and to all sample types except:

- Blank
- Double Blank
- Matrix Blank
- QC
- CC
- Calibration.

The Calibration samples are excluded in order to prevent the lowest and highest calibration points from being pushed out of range by the curve fit residuals.

The outlier is set to High if

$$\text{CalculatedConcentration} > \text{HighestLevelConcentration}$$

where *HighestLevelConcentration* is the level concentration of the highest enabled (LevelEnable) calibration point.

The outlier is set to *Low* if

$$\text{CalculatedConcentration} < \text{LowestLevelConcentration}$$

where *LowestLevelConcentration* is the level concentration of the lowest enabled (LevelEnable) calibration point.

When the outlier is set, the [CalculatedConcentration](#) column is highlighted.

This outlier is always activated unless the batch uses the standard addition quantitation.

## Curve Fit R

This outlier metric is a measure of whether the calibration curve of the current compound has a Pearson correlation coefficient (R) that is below the minimum threshold. This outlier applies to all compound types except ISTD and to all sample types.

This outlier metric is determined by examining the compound's curve fit R value ([CurveFitR](#)) and testing if it lies above [CurveFitMinimumR](#).

Curve fit R values below the minimum are flagged as *Low*.

When the outlier is set, the [CurveFitR](#) column is highlighted.

For the outlier to activate, the following columns must be set in the Quantitation Method Editor:

[CurveFitMinimumR2](#)

## Curve Fit R2

This outlier metric is a measure of whether the calibration curve of the current compound has a coefficient of determination (R<sup>2</sup>) that is below the minimum threshold. This outlier applies to all compound types except ISTD and to all sample types.

This outlier metric is determined by examining the compound's curve fit R<sup>2</sup> value ([CurveFitR2](#)) and testing if it lies above [CurveFitMinimumR2](#).

Curve fit R<sup>2</sup> values below the minimum are flagged as *Low*.

When the outlier is set, the [CurveFitR2](#) column is highlighted.

For the outlier to activate, the following columns must be set in the Quantitation Method Editor:

[CurveFitMinimumR2](#)

## Relative Response Factor

This outlier metric is a measure of whether the relative response factor (RRF) of the current calibration level is close enough to the *average* RRF for this compound. This outlier applies to all compound types except ISTD and to all sample types.

This outlier metric is determined by examining the ratio of each calibration level response factor ([LevelResponseFactor](#)) to the [AverageResponseFactor](#) and determining if the ratio is within the limit defined by the [RelativeResponseFactorMaximumPercentDeviation](#). The outlier is set to as follows:

$$\text{High if } RRF_n > \overline{RRF} \times \left( 1 + \frac{RRFMaximumPercentDeviation}{100} \right)$$

$$\text{Low if } RRF_n < \overline{RRF} \times \left( 1 - \frac{RRFMaximumPercentDeviation}{100} \right)$$

where  $RRF_n$  is the relative response factor for calibration level  $n$ :

$$RRF_n = \frac{LevelResponse_n \times ISTDConc_n}{LevelConc_n \times ISTDResponse_n}$$

and  $\overline{RRF}$  is the average relative response factor over all enabled calibration levels with a non-zero concentration:

$$\overline{RRF} = \frac{1}{N} \sum_{n=1}^N RRF_n$$

For technical reasons, it is not possible to highlight Calibration table columns like [LevelResponseFactor](#). Therefore, when this outlier is set, the [TargetResponse](#) column in the Peak table is highlighted which is the limit column for this outlier.

For the outlier to activate, the following columns must be set in the Quantitation Method Editor: [RelativeResponseFactorMaximumPercentDeviation](#)

Note: This outlier applies only to compounds that have an ISTD.

## Relative Standard Error

This outlier metric is a measure of whether the relative standard error (RSE) across the entire calibration curve is greater than a pre-determined limit. A RSE flagged above the limit can



indicate a poor calibration for the compound. This outlier applies to all compound types except ISTD and to all sample types.

This outlier metric is determined as follows:

Compute [RSE](#) over all enabled calibration points:

$$\%RSE = 100 \times \sqrt{\sum_{i=1}^n \left[ \frac{x'_i - x_i}{x_i} \right]^2 / (n - p)}$$

Where,

$x_i$  = True value of the calibration level  $i$

$x'_i$  = Measured concentration of calibration level  $i$

$p$  = Number of terms in the fitting equation  
(average = 1, linear = 2, quadratic = 3)

$n$  = Number of calibration points

The outlier is set to *High* if

$$\%RSE > \text{RelativeStandardErrorMaximum}$$

When the outlier is set, the [RSE](#) column is highlighted.

For the outlier to activate, the following columns must be set in the Quantitation Method Editor:

[RelativeStandardErrorMaximum](#).

## Response Factor

This outlier metric is a measure of whether the response factor (RF) of the current calibration level is close enough to the *average* response factor for this compound. This outlier applies to all compound types except ISTD and to all sample types.

This outlier metric is determined by comparing each calibration level response factor ([LevelResponseFactor](#)) to the [AverageResponseFactor](#) and testing if the relative deviation is within the limit defined by the [ResponseFactorMaximumPercentDeviation](#). The outlier is set as follows:

$$\text{High if } RF_n > \overline{RF} \times \left( 1 + \frac{RFMaximumPercentDeviation}{100} \right)$$

$$\text{Low if } RF_n < \overline{RF} \times \left( 1 - \frac{RFMaximumPercentDeviation}{100} \right)$$

where  $RF_n$  is the response factor for calibration level  $n$ :

$$RF_n = \frac{(LevelResponse)_n}{(LevelConcentration)_n}$$

and  $\overline{RF}$  is the average response factor over all enabled calibration levels with a non-zero concentration:

$$\overline{RF} = \frac{1}{N} \sum_{n=1}^N RF_n$$

For technical reasons, it is not possible to highlight Calibration table columns like [LevelResponseFactor](#). Therefore, when this outlier is set, the [TargetResponse](#) column in the Peak table is highlighted which is the limit column for this outlier.

For the outlier to activate, the following columns must be set in the Quantitation Method Editor: [ResponseFactorMaximumPercentDeviation](#)

Note: This outlier applies only to compounds that do NOT have an ISTD.

## QC

This set of outliers are grouped together to handle exceptions related to Quality Controls (QC).

## QC

This outlier metric is a measure of whether the current quantitated amount for a compound in a QC sample is within pre-determined limits from the expected amount. This outlier applies to the primary peak of each Target compound in the QC samples. If no primary peak is found, the sample is flagged with a quantitation error message, not with an outlier flag.

This outlier metric is determined by examining the peak's quantitated amount ([CalculatedConcentration](#)) and testing if that amount falls with a pre-defined interval [QCMaximumDeviation](#) from [ExpectedConcentration](#).

The outlier is set to *High* if

$$\text{CalculatedConc} > \text{ExpectedConc} + \text{QCMaximumDeviation}$$

The outlier is set to *Low* if

$$\text{CalculatedConc} < \text{ExpectedConc} - \text{QCMaximumDeviation}$$

When the outlier is set, the [CalculatedConcentration](#) column is highlighted.

For the outlier to activate, the following columns must be set:

[QCMaximumDeviation](#)

[ExpectedConcentration](#)

## QC LCS Recovery

This outlier metric is a measure of whether the recovery of laboratory control standards are within pre-determined limits. This outlier applies to the primary peak of all compounds in all QC samples whose SampleInformation column contains either "LCSA" or "LCSB".

This QC LCS Recovery is calculated as follows and the recovery is deposited to the MatrixSpikePercentRecovery column

$$\text{QC LCS Recovery} = \frac{\text{CalculatedConcentration}}{\text{Level concentration}} \times 100$$

The outlier metric is determined by testing if the QC LCS Recovery falls within the limits.

The outlier is set to *High* if

*QC LCS Recovery* > *QCLCSMaximumRecovery*

The outlier is set to *Low* if

*QC LCS Recovery* < *QCLCSMinimumRecovery*

The SampleInformation value controls the choice of either the LCSA or LCSB limits. In other words, SampleInformation assigned "LCSA" sets LCSA recovery limits, whereas SampleInformation assigned "LCSB" sets LCSB limits.

When the outlier is set, the [MatrixSpikePercentRecovery](#) column is highlighted for all QC samples in a given level.

For the outlier to activate, the following columns must be set:

- SampleInformation column must contain "LCSA" or "LCSB"
- [QCLCSMaximumRecoveryA](#)
- [QCLCSMinimumRecoveryA](#)
- [QCLCSMaximumRecoveryB](#)
- [QCLCSMinimumRecoveryB](#)

## QC Relative Standard Deviation

This outlier metric is a measure of whether the standard deviation of the target response for a set of QC samples at a given level is less than a pre-determined limit. This outlier applies to the primary peak of each Target compound in all QC samples within a given concentration level.

This outlier is computed as follows. For each QC level  $n = 1...N$ , the average, standard deviation of the current compound's [TargetResponse](#) are calculated over all QC samples ( $m=1...M_n$ ) at QC level  $n$ :

$$Avg_n = \frac{1}{M_n} \sum_{m=1}^{M_n} TargetResponse_{m,n}$$

$$SD_n = \sqrt{\frac{1}{M_n - 1} \sum_{m=1}^{M_n} (TargetResponse_{m,n} - Avg_n)^2}$$

For each QC level  $n$  with  $M_n > 1$ , the outlier is set as follows:

*High if  $\%RSD_n > QCMaximumPercentRSD$*

where  $\%RSD_n$  is the relative standard deviation (RSD) of all QC points in level  $n$ , expressed in percent:

$$\%RSD_n = \frac{SD_n}{Avg_n} \times 100$$

When the outlier is set, the [TargetResponse](#) column is highlighted for all QC samples in a given level.

For the outlier to activate, the following columns must be set in the Quantitation Method Editor: [QCMaximumPercentRSD](#).

## CC

This set of outliers are grouped together to handle exceptions related to Continuing Calibration (CC).

### CC Average Response Factor

This outlier metric is a measure of whether the response factor of a compound in a CC sample deviates too much from the average response factor of the initial calibration. This outlier applies to all compounds in CC sample(s).

This outlier metric is determined by computing the relative deviation of the [LevelResponseFactor](#) of a compound in the CC sample from the [AverageResponseFactor](#) for the same compound and comparing the result with the maximum allowed limit [MaximumCCResponseFactorDeviation](#).

The outlier is calculated as follows. The compound's CC response factor deviation between CC and initial calibration is

$$CCResponseFactorDeviation = \left[ 1 - \frac{LevelResponseFactor\_CC}{AverageResponseFactor\_Init} \right] \times 100$$

Here, *LevelResponseFactor\_CC* is the response factor for the compound in the CC sample, *AverageResponseFactor\_Init* is the average response factor for the same compound, and the average is over all enabled Calibration and QC levels.

The outlier is set to *High* either if

$$CCResponseFactorDeviation > MaximumCCResponseFactorDeviation$$

The outlier is set to *Low* if

$$CCResponseFactorDeviation < -MaximumCCResponseFactorDeviation$$

When the outlier is set, the [AverageResponseFactor](#) column is highlighted.

For the outlier to activate, the following columns must be set in the Quantitation Method Editor: [MaximumCCResponseFactorDeviation](#)

## CC ISTD Response Ratio

This outlier metric is a measure of whether the response of an ISTD compound in any sample deviates too much from the previous most recent CC sample or last calibration sample. This outlier applies to the primary peaks of all ISTD compounds in all sample(s).

The outlier is determined by computing the ratio of the [TargetResponse](#) of the primary peak of each ISTD compound in a sample and in the previous CC sample or the last calibration sample, and comparing the result with the limits [CCISTDResponseRatioLimitHigh](#) and [CCISTDResponseRatioLimitLow](#).

The outlier is calculated as follows. The ISTD compound's response ratio to the CC ISTD response is

$$CCISTDResponseRatio = \frac{ISTDResponse}{ISTDResponse\_CC} \times 100$$

where *ISTDResponse\_CC* is the ISTD compound response in the previous most recent CC sample and *ISTDResponse* is the compound response in any sample.

The outlier is set to *High* either if

$$CCISTDResponseRatio > CCISTDResponseRatioLimitHigh$$

The outlier is set to *Low* either if

$$CCISTDResponseRatio < CCISTDResponseRatioLimitLow$$

When the outlier is set, the [CCISTDResponseRatio](#) column is highlighted.

For the outlier to activate, the following columns must be set in the Quantitation Method Editor:

- [CCISTDResponseRatioLimitHigh](#)
- [CCISTDResponseRatioLimitLow](#)

## CC Relative Response Factor

This outlier metric is a measure of whether the relative response factor (RRF) of the compound in a CC is too small. This outlier applies to all Target compounds in CC sample(s).

This outlier metric is determined by computing the relative response factor for each compound in the CC sample and comparing it to the minimum limit defined by [MinimumCCRelativeResponseFactor](#).

The outlier is set to *Low* if:

$$RRF_{CC} < MinimumCCRelativeResponseFactor$$

where  $RRF_{CC}$  is the relative response factor for the CC sample:

$$RRF_{CC} = \frac{LevelResponse_{CC} \times ISTDConc_{CC}}{LevelConc_{CC} \times ISTDResponse_{CC}}$$

For technical reasons, it is not possible to highlight Calibration table columns like [LevelResponseFactor](#). Therefore, when this outlier is set, the [TargetResponse](#) column in the Peak table is highlighted.

For the outlier to activate, the following columns must be set in the Quantitation Method Editor:

- [MinimumCCRelativeResponseFactor](#)

Note: This outlier applies only to compounds that have an ISTD.

## CC Response Ratio

This outlier metric is a measure of whether the response of a target compound in a CC sample deviates too much from the initial calibration. This outlier applies to the primary peaks of all Target compounds in compounds in CC sample(s).

- This outlier metric is determined by computing the ratio of the [TargetResponse](#) of the primary peak of each compound in the CC sample and in the calibration sample at the same concentration level, and comparing the result with the limits [CCResponseRatioLimitHigh](#), [CCResponseRatioLimitLow](#).

The outlier is calculated as follows. The compound's CC response ratio to the initial calibration is

$$CCResponseRatio = \frac{TargetResponse_{CC}}{TargetResponse_{Init}} \times 100$$

where  $TargetResponse_{CC}$  is the compound response in the CC sample and  $TargetResponse_{Init}$  is the compound response in the calibration sample at the same concentration level as the CC sample.



The outlier is set to *High* either if

$$CCResponseRatio > CCResponseRatioLimitHigh$$

The outlier is set to *Low* either if

$$CCResponseRatio < CCResponseRatioLimitLow$$

When the outlier is set, the [TargetResponse](#) column is highlighted.

For the outlier to activate, the following columns must be set in the Quantitation Method Editor:

- [CCResponseRatioLimitLow](#)
- [CCResponseRatioLimitHigh](#)

## CC Retention Time

This outlier metric is a measure of whether the actual retention time of a compound in a CC sample is within the Retention Time (RT) window centered on the expected RT, as defined in the method. This outlier applies to the primary peak of all compound types in CC sample(s).

- This outlier metric is determined by comparing the peak's retention time ([RetentionTime](#) in the Peak table) against the method's retention time ([RetentionTime](#) in the Target Compound table) and testing if the deviation is within the retention time window ([RetentionTimeWindowCC](#)), expressed in minutes.

The outlier is set as follows:

$$\text{High if } RT > RT_{\text{method}} + \frac{1}{2} RT_{\text{WindowCC}}$$

$$\text{Low if } RT < RT_{\text{method}} - \frac{1}{2} RT_{\text{WindowCC}}$$

When the outlier is set, the [RetentionTime](#) column of the Peak table is highlighted.

For the outlier to activate, the following columns must be set in the Quantitation Method Editor:

- [RetentionTimeWindowCC](#)

## CC Time

This outlier metric is a measure of the time elapsed between the acquisition time stamps of any sample and last continuing calibration sample or last calibration sample. This outlier applies to all sample types.

This outlier metric is determined by computing *ElapsedTime*, which is the difference between the acquisition timestamp of any sample and the acquisition timestamp of last CC Sample or last calibration sample, and comparing *ElapsedTime* to the maximum allowed limit [CCMaximumElapsedTimeInHours](#).

*ElapsedTime* is computed as follows:

$$ElapsedTime = TimeStamp(Sample) - TimeStamp(CC)$$

Here *TimeStamp* is the [AcqDateTime](#) column of each sample.

The outlier is set to *High* if

$$ElapsedTime > CCMaximumElapsedTimeInHours$$

When the outlier is set, the [AcqDateTime](#) column of the Sample table is highlighted.

For the outlier to activate, the following batch global parameter must be set to a number greater than 0.

- [CCMaximumElapsedTimeInHours](#)
- 

## Matrix

This set of outliers are grouped together to handle exceptions related to Matrix Spikes.

## Matrix Spike

This outlier metric is a measure of whether the current quantitated amount for a Matrix Spike sample type is above or below pre-determined limits. This outlier applies to the primary peak of each MatrixSpike compound in the samples of type Matrix and MatrixDup. If no primary peak is found, the sample is flagged with a quantitation error message, not with an outlier flag.

This outlier metric is determined by examining the peak's quantitated amount adjusted by the [Multiplier](#) ([FinalConcentration](#)) and testing if that amount falls with the [MatrixSpikeConcentrationLimitLow](#) and [MatrixSpikeConcentrationLimitHigh](#) limits.

---

The outlier is calculated as follows. The amount of the current compound in a matrix sample  $m = 1, 2$  is computed as

$$\text{MatrixAmount}_m = \text{FinalConcentration}_m$$

Here  $\text{FinalConcentration}_1$  is the [FinalConcentration](#) of the current compound in the Matrix Spike sample and  $\text{FinalConcentration}_2$  is the [FinalConcentration](#) of the current compound in the Matrix Duplicate sample. Note that the FinalConcentration in the Matrix Blank sample is not used in computing  $\text{MatrixAmount}_m$ .

### **Note**

Using the Final Concentration takes into account a dilution factor. Hence, diluting the MatrixSpike at any stage of sample preparation is taken into account in measuring against the expected concentration.

The outlier is set to *High* if

$$\text{MatrixAmount}_m > \text{MatrixSpikeConcentrationLimitHigh}$$

The outlier is set to *Low* if

$$\text{MatrixAmount}_m < \text{MatrixSpikeConcentrationLimitLow}$$

When the outlier is set, the [FinalConcentration](#) column is highlighted.

For the outlier to activate, the following must be set:

Compound type is set as MatrixSpike

Sample type is set as Matrix Spike or Matrix Duplicate

[MatrixSpikeConcentrationLimitLow](#)

[MatrixSpikeConcentrationLimitHigh](#)

## Matrix Spike Percent Deviation

This outlier metric is a measure of whether the difference in the quantitated amounts between the Matrix Spike sample and the Matrix Duplicate sample is above or below the pre-determined percent limit. This outlier applies to the primary peak of each MatrixSpike compound in the samples of type Matrix and MatrixDup.

This outlier metric is determined by examining the peak's quantitated amount adjusted by the [Multiplier](#) ([FinalConcentration](#)) compared to the expected amount ([MatrixSpikeConcentration](#)) and testing if [MatrixSpikePercentDeviation](#), the difference in [MatrixSpikePercentRecovery](#) between Matrix Spike and Matrix Duplicate, is outside the [MatrixSpikeMaximumPercentDeviation](#).

The outlier is set to *High* if

$$\text{MatrixSpikePercentDeviation} > \text{MaxPercentDeviation}$$

where

$$\text{MatrixSpikePercentDeviation} = \frac{|FinalConcentration_1 - FinalConcentration_2|}{MatrixSpikeConcentration} \times 100$$

Here  $FinalConcentration_1$  is the [FinalConcentration](#) of the current compound in the Matrix Spike sample and  $FinalConcentration_2$  is the [FinalConcentration](#) of the current compound in the Matrix Duplicate sample.

The SampleInformation value controls the choice of either the Matrix(A) or MatrixB expected concentration and limits. In other words, SampleInformation assigned "MatrixB" sets MatrixB limits and Matrix(B) expected concentration, whereas SampleInformation assigned "MatrixA" sets MatrixA limits and MatrixA expected concentration. Any unmatched value of SampleInformation defaults to Matrix(A).

When the outlier is set, the [MatrixSpikePercentDeviation](#) column is highlighted.

For the outlier to activate, the following must be set:

Compound type is set as MatrixSpike

Sample type is set as Matrix Spike or Matrix Duplicate

Matrix Duplicate sample in same batch

[MatrixSpikeConcentration](#)

[MatrixSpikeMaximumPercentDeviation](#)

## Matrix Group Percent Recovery

This outlier metric is similar to Matrix Spike Percent Recovery but differs from the latter in two ways:

- 1) Matrix Group Percent Recovery applies to all compound types;
- 2) Matrix Group Percent Recovery applies only within a given matrix spike group. A matrix spike group is group of samples that share the same value of the [MatrixSpikeGroup](#) column. Note that a batch may contain multiple matrix spike groups.
- 3) Samples of type Sample can play the role of the Matrix Blank within a matrix spike group.

This outlier metric is calculated separately for each matrix spike group. It is determined by examining the peak's quantitated amount adjusted by the [Multiplier \(FinalConcentration\)](#) compared to the expected [MatrixSpikeConcentration or MatrixSpikeBConcentration](#) and testing if that percent recovery ([MatrixSpikePercentRecovery](#)) falls with the [MatrixSpikePercentRecoveryMinimum](#) and [MatrixSpikePercentRecoveryMaximum](#) limits or the [MatrixSpikeBPercentRecoveryMinimum](#) and [MatrixSpikeBPercentRecoveryMaximum](#) limits. The outlier is calculated as follows. For the Matrix and MatrixDup samples, the current compound's percent recovery ([MatrixSpikePercentRecovery](#)) is

$$\text{MatrixRecovery} = \frac{\text{FinalConcentration}_m - \text{MatrixBlankConcentration}}{\text{MatrixSpikeConcentration}} \times 100$$

Here  $\text{FinalConcentration}_m$  is the [FinalConcentration](#) of the current compound in the Matrix sample or in the MatrixDup sample;  $\text{MatrixBlankConcentration}$  is the [FinalConcentration](#) of the current compound in the MatrixBlank sample or in the target Sample that belongs to the same matrix spike group.

The SampleInformation value controls the choice of either the Matrix(A) or MatrixB expected concentration and limits. In other words, SampleInformation assigned "MatrixB" sets MatrixB limits and Matrix(B) expected concentration, whereas SampleInformation assigned "MatrixA" sets MatrixA limits and MatrixA expected concentration. Any unmatched value of SampleInformation defaults to Matrix(A).

Membership in a matrix spike group is subject to the following assumptions/requirements:

1. A matrix spike group can contain one or more sample of type Sample or MatrixBlank. This is the "unspiked" sample. If no "unspike" sample present in the matrix spike group, MatrixBlankConcentration is considered as zero.
2. A matrix spike group must contain at least one sample of type Matrix or MatrixDup. These are the "spiked" samples.
3. If a matrix spike group contains multiple "unspiked" samples, only the first "unspiked" sample is used; the others are ignored.
4. Any group that does not satisfy the assumptions 1) and 2) is ignored.
5. The Matrix Spike Group Recovery outlier is calculated for each "spiked" sample in the group.

The outlier is set to *High* if

$MatrixRecovery > MatrixSpikePercentRecoveryMaximum$

The outlier is set to *Low* if

$MatrixRecovery < MatrixSpikePercentRecoveryMinimum$

When the outlier is set, the [MatrixSpikePercentRecovery](#) column is highlighted.

For the outlier to activate, the following must be set:

- Sample type is set as Matrix or MatrixDup
- Matrix, MatrixDup, and MatrixBlank samples in the same batch
- [MatrixSpikeConcentration](#)
- [MatrixSpikePercentRecoveryMinimum](#)
- [MatrixSpikePercentRecoveryMaximum](#)

## Matrix Spike Percent Recovery

This outlier metric is a measure of whether the ratio of the current quantitated amount to expected amount for a Matrix Spike sample is above or below pre-determined pre-defined limits. This criterion is often used to measure the fixed boundaries from the expected recovery for a Matrix Spike compound. This outlier applies to the primary peak of each MatrixSpike compound in the samples of type Matrix and MatrixDup. If no primary peak is found, the sample is flagged with a quantitation error message, not with an outlier flag.

This outlier metric is determined by examining the peak's quantitated amount adjusted by the [Multiplier \(FinalConcentration\)](#) compared to the expected [MatrixSpikeConcentration](#) and testing if that percent recovery ([MatrixSpikePercentRecovery](#)) falls with the [MatrixSpikePercentRecoveryMinimum](#) and [MatrixSpikePercentRecoveryMaximum](#) limits.

The outlier is calculated as follows. For the Matrix Spike and the Matrix Duplicate samples, the current compound's percent recovery ([MatrixSpikePercentRecovery](#)) is

$MatrixRecovery =$

$$\frac{FinalConcentration_m - MatrixBlankConcentration}{MatrixSpikeConcentration} \times 100$$

Here  $FinalConcentration_m$  is the [FinalConcentration](#) of the current compound in the Matrix Spike sample or in the Matrix Duplicate sample;  $MatrixBlankConcentration$  is the [FinalConcentration](#) of the current compound in the Matrix Blank sample.

The outlier is set to *High* if

$MatrixRecovery > MatrixSpikePercentRecoveryMaximum$

The outlier is set to *Low* if

$$\text{MatrixRecovery} < \text{MatrixSpikePercentRecoveryMinimum}$$

When the outlier is set, the [MatrixSpikePercentRecovery](#) column is highlighted.

For the outlier to activate, the following must be set:

- Compound type is set as MatrixSpike
- Sample type is set as Matrix or MatrixDup
- A single triplet of Matrix, MatrixDup, and MatrixBlank samples in the same batch
- [MatrixSpikeConcentration](#)
- [MatrixSpikePercentRecoveryMinimum](#)
- [MatrixSpikePercentRecoveryMaximum](#)
- MatrixGroup is not assigned



# Surrogate

This set of outliers are grouped together to handle exceptions related to Surrogates.

## Surrogate

This outlier metric is a measure of whether the current quantitated amount for a surrogate compound type is above or below pre-determined limits. This outlier applies to the primary peak of each Surrogate compound in all sample types except Blank and DoubleBlank. If no primary peak is found, the sample is flagged with a quantitation error message, not with an outlier flag.

This outlier metric is determined by examining the peak's quantitated amount ([FinalConcentration](#)) adjusted by the [Multiplier](#) and testing if that amount falls within the [SurrogateConcentrationLimitLow](#) and [SurrogateConcentrationLimitHigh](#) limits.

The outlier is set to *High* if

$$\text{SurrogateAmount} > \text{SurrogateConcentrationLimitHigh}$$

The outlier is set to *Low* if

$$\text{SurrogateAmount} < \text{SurrogateConcentrationLimitLow}$$

Here *SurrogateAmount* is the [FinalConcentration](#) of the current surrogate compound.

When the outlier is set, the [FinalConcentration](#) column is highlighted.

For the outlier to activate, the following must be set in the Quantitation Method Editor:

- Compound type is Surrogate
- [SurrogateConcentrationLimitLow](#)
- [SurrogateConcentrationLimitHigh](#)

## Surrogate Percent Recovery

This outlier metric is a measure of whether the current quantitated amount for a surrogate compound type is above or below pre-determined limits. This criterion is often used to measure the fixed boundaries from the expected recovery for a surrogate compound. This outlier applies to the primary peak of each Surrogate compound in all sample types except DoubleBlank. If no primary peak is found, the sample is flagged with a quantitation error message, not with an outlier flag.

This outlier metric is determined by examining the peak's quantitated amount adjusted by the [Multiplier](#) ([FinalConcentration](#)) compared to the expected [SurrogateConcentration](#) and testing if the ratio falls with the [SurrogatePercentRecoveryMinimum](#) and [SurrogatePercentRecoveryMaximum](#) limits.

The outlier is calculated as follows. The current surrogate compound's percent recovery ([SurrogatePercentRecovery](#)) is

$$\text{SurrogateRecovery} = \frac{\text{FinalConcentration}}{\text{SurrogateConcentration}} \times 100$$

The outlier is set to *High* if

$$\text{SurrogateRecovery} > \text{SurrogatePercentRecoveryMaximum}$$

The outlier is set to *Low* if

$$\text{SurrogateRecovery} < \text{SurrogatePercentRecoveryMinimum}$$

When the outlier is set, the [SurrogatePercentRecovery](#) column is highlighted.

For the outlier to activate, the following must be set in the Quantitation Method Editor:

Compound type is Surrogate

[SurrogateConcentration](#)

[SurrogatePercentRecoveryMinimum](#)

[SurrogatePercentRecoveryMaximum](#)

# Response Check

This set of outliers are grouped together to handle exceptions related to Response Check.

## Response Check

This outlier metric is a measure of whether the Response Check sample compounds pass the minimum response criterion. This outlier applies to the primary peak of every Target compound in samples of type ResponseCheck. If no primary peak is found, the sample is flagged with a quantitation error message, not with an outlier flag.

This outlier metric is determined by comparing the [TargetResponse](#) column of the primary peak of each compound in the Response Check sample against [ResponseCheckMinimum](#).

The outlier is set to *Low* if

$$\textit{TargetResponse} < \textit{ResponseCheckMinimum}$$

When the outlier is set, the [TargetResponse](#) column is highlighted.

For the outlier to activate, the following columns must be set in the Quantitation Method Editor:

- [ResponseCheckMinimum](#)

# Mass

This set of outliers are grouped together to handle exceptions related to Mass.

## Library Match Score

This outlier metric is a measure of the correlation between the extracted spectrum and the reference library spectrum. The reference library can be generated from a high level calibration sample or from an existing library.

ReferenceLibraryMatchScore is an indicator of the quality of the match between the sample spectrum and the reference library spectrum. A score of 100 means a perfect match.

The outlier is set to *Low* if

$$\text{ReferenceLibraryMatchScore} < \text{LibraryMatchScoreMinimum}$$

When the outlier is set, the [ReferenceLibraryMatchScore](#) column of the Peak table is highlighted.

For the outlier to activate, the following columns must be set in the Quantitation Method Editor:

- [LibraryMatchScoreMinimum](#)

## Mass Accuracy

This outlier metric is a measure of mass difference between expected MZ and the actual centroided spectral mass against a user-defined limit. This outlier applies to the primary peak of all compound types and all sample types.

The Mass Accuracy is the mass assignment of the averaged scan spectra across the target or qualifier chromatographic peak. This averaged spectrum does take into account saturation if `SpectrumPercentSaturationThreshold` is specified. A poor Mass Accuracy metric indicates a mass drift which can arise from tune, or other effects.

The acceptable mass accuracy is defined as within the [MassAccuracyLimit](#). [MassAccuracy](#) is calculated as the difference between the expected MZ and the most abundant MZ peak found within the range [[MZ](#) - [MZExtractionWindowFilterLeft](#), [MZ](#)+[MZExtractionWindowFilterRight](#)], it is measured in units as determined by the [MZExtractionWindowUnits](#) setting (Thomason, PPM, Percent).

The outlier is set to *High* if

$$\text{MassAccuracy} > +\text{MassAccuracyLimit}$$

The outlier is set to *Low* if

$$\text{MassAccuracy} < -\text{MassAccuracyLimit}$$

When the outlier is set, the [MassAccuracy](#) column of the Target Compound table is highlighted.

For the outlier to activate, the following columns must be set in the Quantitation Method Editor:

- [MassAccuracyLimit](#)

## Mass Match Score

This outlier metric is a measure of the probability that the observed isotope spectrum pattern matches the synthesized isotope pattern. This outlier applies to the primary peak of all compound types and all sample types.

Mass match score is defined as weighted aggregate of the three individual metrics including mass accuracy score, mass abundance score and mass spacing score. In this computation, the weighting factors are taken from the accurate mass metrics parameters configuration file `AccuMassMetricsParams.xml`, which is located under the bin directory. The default values are

$$W_{mass} = 100.0$$

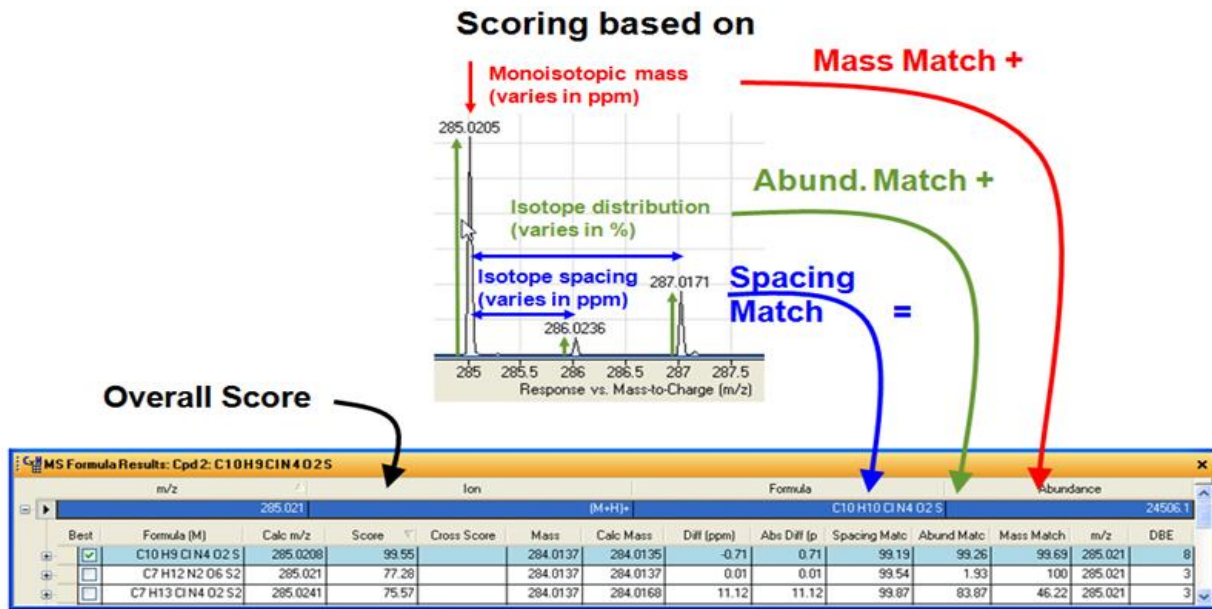
$$W_{abundance} = 60.0$$

$$W_{spacing} = 50.0$$

The equation for computing the overall score is then

*MassMatchScore*

$$= \frac{W_{mass} * MassAccuracyScore + W_{abundance} * MassAbundanceScore + W_{spacing} * MassSpacingScore}{W_{mass} + W_{abundance} + W_{spacing}}$$



The outlier is set to *Low* if

$$MassMatchScore < MassMatchScoreMinimum$$

When the outlier is set, the [MassMatchScore](#) column of the Peak table is highlighted.

For the outlier to activate, the following columns must be set in the Quantitation Method Editor:

- [MassMatchScoreMinimum](#)

## Alternative Peak

This outlier metric is a measure of goodness of fit of the primary peak against certain criteria [AlternativePeakCriteria](#). When the AlternativePeakCriteria is DeconvolutedLibraryMatchScore, component spectrum of each alternative peak is compared against the reference library, and library match scores are calculated. If any alternative peak has better matched component, [AlternativePeakRTDiff](#) is calculated as the RT difference between the primary peak and the alternative peak.

The outlier is set to *High* if

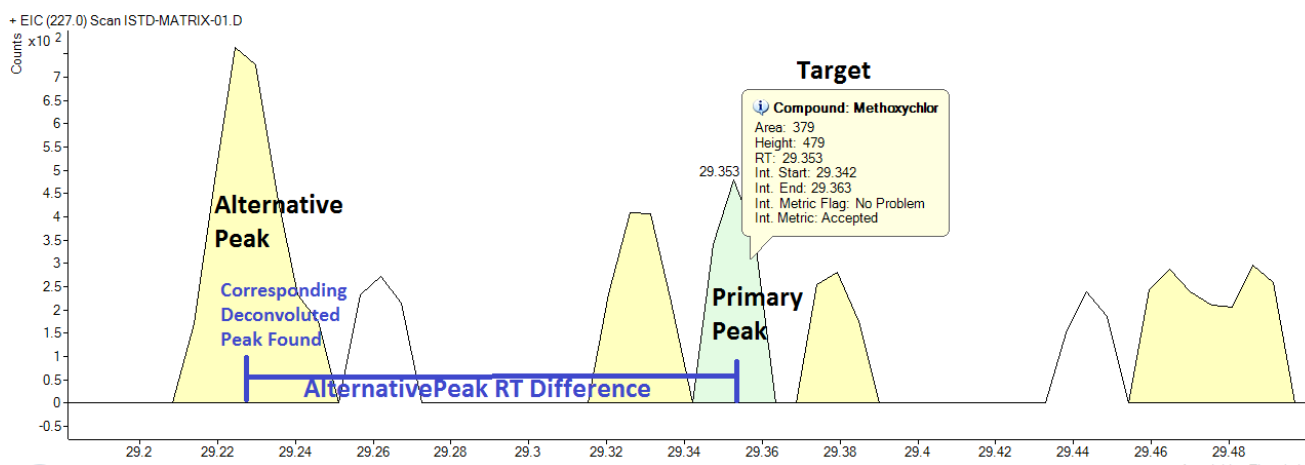
$$AlternativePeakRTDiff > 0$$

Which indicates the alternative peak with better library match score is on the right side of the current primary peak.

And the outlier is set to *Low* if

$$\text{AlternativePeakRTDiff} < 0$$

Which indicates the alternative peak with better library match score is on the left side of the current primary peak.



For the outlier to activate, the following columns must be set in the Quantitation Method Editor:

- [AlternativePeakCriteria](#)

## Saturation Recovery

This outlier metric is an indicator of whether an accurate mass signal is recovered successfully or not by Feature Detection aka "SureMass extrapolation". Feature Detection offers extended dynamic range by signal processing. In some boundary condition cases, the existing signal is not sufficient to recover, so we need to notify the analyst. Notifying the analyst of a possible false negative often results in re-injecting the sample with dilution in order to see a signal which is within the limits.

The outlier is computed by comparing the ratio of the restored feature peak height to the original feature peak height. The feature peak and recovery of feature peak are determined by the feature detection algorithm for accurate mass data. [SaturationRecoveryRatio](#) indicates the status of feature recovery:

Saturation Recovery Ratio	Recovery Status
Null	Feature is not saturated
0	Feature is saturated and not recovered
>0	Feature is saturated but recovered

The outlier is set to *High* if feature is saturated and not recovered, i.e.

$$\text{SaturationRecoveryRatio} = 0$$

Saturation Recovery outlier is automatically enabled when SureMass global is set.

# Custom

This set of outliers are grouped together to handle exceptions related to Custom Calculations.

## Custom Calculation

This outlier metric is a measure of whether the result of a user custom calculation falls within the user-defined limits This outlier applies to all target compounds in all sample types.

This outlier metric is determined by comparing the value of the [UserCustomCalculation](#) column in the Target Compound table, treated as a double-precision floating-point number, against the user-defined limits [UserCustomCalculationLimitLow](#) and [UserCustomCalculationLimitHigh](#).

The outlier is set to *High* if

$$UserCustomCalculation > UserCustomCalculationLimitHigh$$

The outlier is set to *Low* if

$$UserCustomCalculation < UserCustomCalculationLimitLow$$

When the outlier is set, the [UserCustomCalculation](#) column of the Target Compound table is highlighted.

For the outlier to activate, the following columns must be set in the Quantitation Method Editor:

- [UserCustomCalculationLimitLow](#)
- [UserCustomCalculationLimitHigh](#)