SkylineDocument

Name	Description	Type
Molecule Lists	The top level set of the groupings of all of the molecules in a Skyline document.	List of Molecule List
Replicates	Replicates	List of Replicate

Molecule List

Name	Description	Type
Molecules	The molecules in a Molecule List.	List of Molecule
Molecule List Results	Molecule List Results	Map of ResultKey to Molecule List Result
Molecule List Name	The name of the molecule list.	String
Protein Description	When proteins are imported into Skyline through public FASTA sequence files, a Protein Description is provided. You can see the Protein Description also when you hover over the protein name in the peptide tree view.	String
Protein Accession	Protein Accession	String
Protein Preferred Name	Protein Preferred Name	String
Protein Gene	Protein Gene	String
Protein Species	Protein Species	String

Protein Sequence	When proteins are imported into Skyline through public FASTA sequence files the full protein sequence is accessible. You can see the protein sequence also when you hover over the protein name in the peptide tree view.	String
Auto Select Molecules	If true, then Skyline will automatically add or remove molecules from the Molecule List based on the current settings.	Boolean
Protein Sequence Coverage	The fraction of amino acids in the protein sequence which could be part of one or more of the sequences of the child peptides.	Double
Molecule List Note	A free text note associated with the molecule list.	String
Molecule List Locator	Unique identifier of the molecule list within the document. This begins with "MoleculeGroup:".	String

Replicate

Name	Description	Type
Replicate Name	The replicate name assigned to the data during import.	String
Files	Files	List of Result File
Sample Type	Type of the sample. One of the following: Unknown (sample being measured) Standard (external standard containing a known amount of analyte to be used in calibration curve) Quality Control (containing a known amount of analyte to verify calibration) Solvent Blank Double Blank	Sample Type
Analyte Concentration	Known quantity of analyte that was spiked into the external or quality control standard.	Double

Sample Dilution Factor	The amount by which the sample was diluted before being analyzed. External standards typically have a dilution factor of 1, and unknown samples may have been diluted by a factor greater than 1 in order to bring them into the quantifiable range for the instrument.	Double
Batch Name	Name of the batch that this replicate belongs to. The calibration curve for a particular replicate will be calculated using the subset of external standards with the same batch name.	String
Replicate Locator	Unique identifier of the replicate within the document. This is always "Replicate:/" followed by the name of the replicate.	String

Molecule

Name	Description	Type
Precursors	Precursors	List of Precursor
Molecule Results	The results associated with the molecule.	Map of ResultKey to Molecule Result
Molecule List	A grouping of molecules in a Skyline document.	Molecule List
Peptide Sequence	Amino acid sequence of the peptide.	String
Peptide Sequence Length	Amino acid count in the sequence of the peptide.	Int32
Peptide Modified Sequence	Amino acid sequence annotated with only structural modification delta masses (e.g. AC [+57]GR).	ProteomicSequence

Name	Description	Type

	Peptide Modified Sequence Monoisotopic Masses	The modified sequence of the peptide where modifications are referred to by their monoisotopic masses, e.g. "C[+57.021464]".	String
	Peptide Modified Sequence Average Masses	The modified sequence of the peptide where modifications are referred to by their average masses, e.g. "C[+57.05162]".	String
	Peptide Modified Sequence Three Letter Codes	The modified sequence of the peptide where modifications are referred to by their three letter codes, e.g. "C[CAM]". If the modification does not have a three letter code, then its full name is used instead.	String
	Peptide Modified Sequence Full Names	The modified sequence of the peptide where modifications are referred to by their full names, e.g. "C[Carbamidomethyl (C)]".	String
	Peptide Modified Sequence Unimod Ids	The modified sequence of the peptide where modifications are referred to by their unimod id, e.g. "C(unimod:4)". If the modification does not have a unimod id, then its full name is used instead.	String
Molecule Name	A general name that may be assigned to a molecule in its neutral, unlabeled form.		String
Molecule Formula	An atomic chemical formula for the neutral, unlabeled molecule to be measured in a mass spectrometer.		String
Standard Type	Standard Type		Standard Type
Previous Aa	Previous Aa		Char

Next Aa	Next Aa	Char
First Position	The position of the first (N-terminal) amino acid of the peptide within its containing protein sequence, or #N/A if no protein sequence is available.	Int32
Last Position	The position of the last (C-terminal) amino acid of the peptide within its containing protein sequence, or #N/A if no protein sequence is available	Int32
Missed Cleavages	The number of missed cleavage sites in the peptide sequence	Int32
Retention Time Calculator Score	The raw score for the peptide from the current retention score calculator, if one is used (e.g. SSRCalc or iRT score)	Double
Predicted Retention Time	The retention time predicted by a retention time regression between a set of measured results and a retention time calculator (currently only SSRCalc 3.0 is available), or #N/A if no retention time regression has been assigned.	Double
Average Measured Retention Time	The average peptide retention time over all replicates	Double
Explicit Retention Time	The exact predicted retention time (in minutes) to be used for a target, overriding all other methods of prediction.	Double
Explicit Retention Time Window	The exact desired retention time window (in minutes) to be used for a target, overriding all other settings used to derive this value.	Double
Normalization Method	Override of the normalization method to use with this particular molecule for absolute quantification and group comparisons.	Normalization Method

Molecule Note	A free text note associated with the molecule.	String
Molecule Locator	Unique identifier of the molecule within the document. This begins with "Molecule:".	String
Internal Standard Concentration	Quantity of internal standard in the sample.	Double
Concentration Multiplier	Value to multiply the replicate's "analyte concentration" by in order to get the specific concentration of the specific peptide or molecule.	Double
Calibration Curve	Calibration Curve that was calculated using Replicates whose Sample Type was "Standard" and that had an "Analyte Concentration" specified.	Calibration Curve
Figures Of Merit	The limits of detection and quantification for the peptide or molecule. The method for calculating these quantities can be chosen on the Quantification tab of the Peptide Settings.	Figures Of Merit
InChiKey	Standardized molecular identifier	String
CAS	Standardized molecular identifier	String
HMDB	Standardized molecular identifier	String
InChI	Standardized molecular identifier	String
SMILES	Standardized molecular identifier	String
KEGG	Standardized molecular identifier	String
Auto Select Precursors	If true, then Skyline will automatically add or remove precursors based on the Transition Settings Filter, spectral library, etc.	Boolean
Attribute Group	Affects the grouping of peptides or molecules	String

ID	in the calculation of Attribute Area Proportion.	

Calibration Curve

Name	Description	Type
Slope	Coefficient of the linear term in the fitted curve or line.	Double
Intercept	Y-intercept in the fitted line or curve	Double
Turning Point	For bilinear regressions, the X-coordinate where the two lines intersect.	Double
Point Count	Number of data points that were used in the curve fit.	Int32
Quadratic Coefficient	Coefficient of the x-squared term in a quadratic regression.	Double
R Squared	Coefficient of determination	Double
Error Message	Text of the error message, if any, which occurred while trying to calculate this value.	String

Figures Of Merit

Name	Description	Type
Limit Of Detection	The lower concentration limit at which the analyte can be reliably distinguished from a blank. The options about for calculating the lower limit of detection can be specified on the Quantification tab of the Peptide Settings.	Double
Limit Of Quantification	The lower concentration limit where the analyte is said to be quantifiable. The options for determining this value can be specified on the Quantification tab of the Peptide Settings.	Double

Molecule List Result

Name	Description	Type
Replicate	Replicate	Replicate
Molecule List Abundance	A number representing the abundance of the molecule list. This number is obtained by averaging the normalized areas of all of the transitions under this Molecule List. The areas are normalized according to the Normalization Method specified in the Molecule Quantification settings. The Molecule List Abundance will be blank if any transitions have missing values in this replicate, unless the normalization method is ratio to a label.	Double

ResultKey

Name	Description	Type
Replicate Index	Replicate Index	Int32
Replicate Name	The replicate name assigned to the data during import.	String
File Index	File Index	Int32

Result File

Name	Description	Type
Replicate	Replicate	Replicate
File Name	The name of the file from which the data was imported	String
File Path	The full path and file name of the file from which the data was imported.	String
Sample Name	The sample name, if the data was imported from a multi-sample WIFF file, or the file name again for other file types.	String

Modified Time	Last time and date at which the original mass spectrometer file was modified on disk	DateTime
Acquired Time	Last time and date at which the mass spectrometer began acquiring this replicate data. Or #N/A if the file was imported with a version older than 1.1.	DateTime
Explicit Global Standard Area	Value to use when calculating "ratio to global standards". Use this when you want to normalize peak areas in a particular replicate by dividing by a value that you calculated outside of Skyline.	Double
Total Ion Current Area	Integral of the total ion current over the entire run.	Double
Ion Mobility Units	Units for ion mobility used in chromatogram extraction.	eIonMobilityUnits
Result File Locator	Unique identifier of the result file within the document. This begins with "ResultFile:/" followed by the replicate name. This usually ends with the result filename, but may have additional attributes such as the full path if the filename is not unique within the replicate.	String
Sample Id	A free text identifier for referring to a sample (which may be shared among multiple files). Read from the "sample id" attribute in an imported result file	String
Instrument Serial Number	The instrument serial number read from an imported result file	String
Median Peak Area	The median transition peak area of transition results in the particular result file. This median peak area is used when the normalization method is "Equalize Medians". If there is an internal standard label type, then the median peak area is calculated using only the peak areas from transitions whose precursor's label type is an internal standard. If there are no internal standard peak areas, then the median transition peak area is	Double

	calculated from all transition peak areas.	
Normalization Divisor	Number which observed values are divided by when using the default normalization method. The default normalization method is specified on the Quantification tab of the Peptide or Molecule settings dialog.	Double

Precursor

Name	Description	Type
Molecule	Molecules belong to Molecule Lists and contain Percursors.	Molecule
Transitions	Transitions	List of Transition
Precursor Results	Precursor Results	Map of ResultKey to Precursor Result
Precursor Results Summary	Precursor Results Summary	PrecursorResultSummary
Precursor Charge	The charge associated with the precursor ion.	Int32
Isotope Label Type	A label type name associated with the precursor ion (light/heavy), indicating which isotope modifications are applied	Isotope Label Type
Precursor Neutral Mass	Neutral mass of the precursor in Daltons	Double
Transition Count	Number of transitions under this precursor.	Int32
Precursor Ion Name	The name of the precursor.	String

Precursor Ion Formula	The formula of the precursor ion.	String
Precursor Neutral Formula	The formula of the precursor ion. This is deprecated and "PrecursorIonFomula" should be used instead.	String
Precursor Adduct	The adduct which is applied to the molecule to make the precursor.	String
Precursor Mz	The mass to charge ratio (m/z) of the precursor ion.	Double
Collision Energy	Collision Energy for the precursor ion according to instrument/vendor specific default collision energy equation within Skyline	Double
Declustering Potential	Declustering Potential for the precursor ion according to instrument/vendor specific default declustering potential equation within Skyline	Double
Modified Sequence	Peptide sequence including any amino acid modifications such as cysteine alkylation. (example: AGLC[+57]QTFVYGGC[+57]R)	ProteomicSequence

Name	Description	Type
Modified Sequence Monoisotopic Masses	The modified sequence of the precursor where modifications are referred to by their monoisotopic masses, e.g. "C[+57.021464]".	String
Modified Sequence Average Masses	The modified sequence of the precursor where modifications are referred to by their average masses, e.g. "C[+57.05162]".	String

	Modified Sequence Three Letter Codes	The modified sequence of the precursor where modifications are referred to by their three letter codes, e.g. "C[CAM]". If the modification does not have a three letter code, then its full name is used instead.	String
	Modified Sequence Full Names	The modified sequence of the precursor where modifications are referred to by their full names, e.g. "C[Carbamidomethyl (C)]".	String
	Modified Sequence Unimod Ids	The modified sequence of the precursor where modifications are referred to by their unimod id, e.g. "C(unimod:4)". If the modification does not have a unimod id, then its full name is used instead.	String
Precursor Explicit Collision Energy	The exact desired collision energy to be used in SRM methods or transitions lists for a target, overriding all model or optimization library values. May in turn be overridden by per-transition Explicit Collision Energy.	Double	
Explicit Compensation Voltage	The exact desired compensation voltage (ion mobility filter) to be used in SRM methods or transitions lists for a target, overriding all model or optimization library values.	Double	
Explicit Ion Mobility	The ion mobility value of the center of the filter window used when extracting chromatograms	Double	
Explicit Ion Mobility Units	The units of the Explicit Ion Mobility values.	String	

Explicit Collisional Cross Section	The exact desired collisional cross section (in square angstroms) to be converted to ion mobility and used in extracting chromatograms from ion mobility mass spectra, overriding all model values.	Double
Precursor Concentration	The concentration at which this precursor was spiked into the sample. This is used for generating Isotopolog Response Curves.	Double
Library Ion Mobility	The ion mobility information for the precursor from the ion mobility library	IonMobilityObject

Name	Description	Type
Library Ion Mobility Value	The ion mobility of the precursor from the ion mobility library	Double
Library Ion Mobility Units	The units of the Library Ion Mobility Value	String
Library Collision Cross Section	The collision cross section for the precursor from the ion mobility library	Double
Library Ion Mobility High Energy Offset	The high energy offset for the precursor from the ion mobility library	Double

Spectrum Filter	Extra criteria that spectra must pass to be included in the extracted ion chromatogram	String
Precursor Note	A free text note associated with a precursor by clicking Edit Note on the Edit menu	String
Library Name	The name of a MS/MS spectral library, if a MS/MS spectral library spectrum is associated with the precursor ion.	String

Library Type	The type of MS/MS spectral library (BiblioSpec, GPM, NIST), if a MS/MS spectral library spectrum is associated with the precursor ion.	String
Library Probability Score	The probability score assigned to this match in the input files used to build the spectral library.	Double
Library Score1	Raw peptide library score that may or may not be used to rank among precursors of a protein.	Double
Library Score2	Raw peptide library score that may or may not be used to rank among precursors of a protein.	Double
Library Score3	Raw peptide library score that may or may not be used to rank among precursors of a protein.	Double
Is Decoy	True if this is a decoy precursor.	Boolean
Decoy Mz Shift	Shift in m/z applied to the precursor to create the decoy m/z	Int32
Auto Select Transitions	If true, then Skyline will automatically add or remove transitions from the precursor depending on the Transition Settings Filter, spectral library, etc.	Boolean
Target Qualitative Ion Ratio	The average of the Qualitative Ion Ratio values across all of the external standard replicates that have not been excluded from calibration.	Double
Precursor Locator	Unique identifier of the precursor within the document. This will begin with "Precursor:" and usually ends with the precursor's label type followed by its adduct.	String

PrecursorResultSummary

Name	Description	Type
Best Retention Time	The RetentionTime value of the transition with the highest maximum intensity for the precursor.	RetentionTimeSummary
Detection Q Value	A false discovery rate (FDR) score assigned to each chosen target peak after applying a mProphet model.	DetectionQValueSummary

Name	Description	Type
Min Best Retention Time	Minimum of the precursor BestRetentionTime values	Double
Max Best Retention Time	Maximum of the precursor BestRetentionTime values	Double
Range Best Retention Time	The difference between MaxBestRetentionTime and MinBestRetentionTime, which can be used to gauge the spread of retention times measured.	Double
Mean Best Retention Time	Mean of the precursor BestRetentionTime values.	Double
Stdev Best Retention Time	Standard deviation of the precursor BestRetentionTime values.	Double
Cv Best Retention Time	Coefficient of variation (CV) of the precursor BestRetentionTime values.	Double

Name	Description	Type
Min Detection Q Value	A minimum of the false discovery rate (FDR) score assigned to each chosen target peak after applying a mProphet model.	Double
Max Detection Q Value	A maximum of the false discovery rate (FDR) score assigned to each chosen target peak after applying a mPro phet model.	Double
Median Detection Q Value	A median of the false discovery rate (FDR) score assigned to each chosen target peak after applying a mProphet model.	Double

Max Fwhm	The maximum full width at half max (FWHM) of the transitions for the precursor.	FwhmSummary

Name	Description	Type
Mean Max Fwhm	Mean of the precursor MaxFwhm (peak width) values.	Double
Stdev Max Fwhm	Standard deviation of the precursor MaxFwhm (peak width) values.	Double
Cv Max Fwhm	Coefficient of variation (CV) of the precursor MaxFwhm (peak width) values.	Double

Total Area	The summed Area values of all individual transitions for the particular precursor.	AreaSummary

Name	Description	Type
Mean Total Area	Mean of the precursor TotalArea values.	Double

	Stdev Total Area	Standard deviation of the precursor TotalArea values	Double
	Cv Total Area	Coefficient of variation (CV) of the precursor TotalArea values	Double
Total Area Ratio	The ratio of the TotalArea of this precursor to the first internal standard label type, before version 0.7 this was always light/heavy, and appeared on the heavy precursor.	AreaRatioSummary	

Name	Description	Type
Mean Total Area Ratio	Mean of the precursor TotalAreaRatio values.	Double
Stdev Total Area Ratio	Standard deviation of the precursor TotalAreaNormalized values.	Double
Cv Total Area Ratio	Coefficient of variation (CV) of the precursor TotalAreaRatio values	Double

Total Area Normalized	The TotalArea normalized to the sum of the TotalArea values for all peptide precursors in the document	AreaNormalizedSummary

Name	Description	Type
Mean Total Area Normalized	Mean of the precursor TotalAreaNormalized values	Double
Stdev Total Area Normalized	Stdev Total Area Normalized	Double
Cv Total Area	Coefficient of variation (CV) of the	Double

	Normalized	precursor TotalAreaNormalized values.	
Max Height	Max Height		AreaSummary

Name	Description	Type
Mean Max Height	Mean Max Height	Double
Stdev Max Height	Stdev Max Height	Double
Cv Max Height	Cv Max Height	Double

Molecule Result

Name	Description	Type
Molecule Peak Found Ratio	Molecule Peak Found Ratio	Double
Molecule Retention Time	The average of the Best Retention Time values for the precursors in a particular replicate.	Double
Predicted Result Retention Time	Peptide retention time for each replicate run.	Double
Ratio To Standard	Peptide area ratio of light to heavy	Double
Best Replicate	True if this replicate has the highest overall peptide peak score.	Boolean
Modified Area Proportion	The normalized area of this peptide result divided by the sum of all peptide results in this protein and replicate that have the same unmodified sequence.	Double

Attribute Area Proportion	The ratio of the normalized area to the sum of the normalized areas of all of the other peptides or molecules in the document that have the same Attribute Area Proportion.	Double
Result File	Result File	Result File
Molecule List Result	Molecule List Result	Molecule List Result
Exclude From Calibration	Whether the results in the replicate should be excluded from the peptide's calibration curve calculation.	Boolean
Quantification	Values related to using the calibration curve or normalization method to quantify the analyte.	QuantificationResult
Replicate Calibration Curve	The calibration curve made using the replicates that have the same Batch Name as this replicate. If the Precursor Concentration is specified on any of the Precursors in this Peptide then the Calibration Curve will be an isotopolog response curve.	Calibration Curve

Name	Description	Type
Replicate Slope	The slope of the Replicate Calibration Curve	Double
Replicate Intercept	The intercept of the Replicate Calibration Curve	Double
Replicate Turning Point	The bilinear turning point on the Replicate Calibration Curve	Double
Replicate Point	The number of data points that	Int32

	Count	were fitted on the Replicate Calibration Curve	
	Replicate Quadratic Coefficient	The coefficient of the x-squared term on the Replicate Calibration Curve	Double
	Replicate R Squared	The coefficient of determination on the Replicate Calibration Curve	Double
	Replicate Error Message	Text of the error message, if any, which occurred while trying to fit the Replicate Calibration Curve	String
Batch Figures Of Merit	Figures of merit calculated using the subset of external standard replicates that have the same Batch Name as this replicate.	Figures Of Merit	

Name	Description	Type
Batch Limit Of Detection	Lower limit of detection calculated using the subset of external standard replicates that have the same Batch Name as this replicate.	Double
Batch Limit Of Quantification	Lower limit of quantification calculated using the subset of external standard replicates that have the same Batch Name as this replicate.	Double

Explicit Analyte Concentration	The concentration of this particular molecule or peptide in this particular replicate. If the Explicit Analyte	Double

	Concentration is not specified then the concentration of the analyte is assumed to be the Analyte Concentration from the Replicate times the Concentration Multiplier of the Peptide or Molecule.	
Molecule Result Locator	Unique identifier of the Molecule Result within the document. This will begin with "MoleculeResult:" and will contain the molecule name and the replicate name.	String
RatioLightToHeavy		Double
DotProductLightToHeavy		Double

Transition

Name	Description	Type
Precursor	Precursor	Precursor
Transition Results	Transition Results	Map of ResultKey to Transition Result
Transition Results Summary	Transition Results Summary	TransitionResultSummary
Product Charge	Charge (z) of the product ion.	Int32
Product Neutral Mass	Neutral mass of the product ion peptide fragment in Daltons.	Double
Product Mz	The mass to charge ratio (m/z) of the product ion.	Double
Fragment Ion	The name of the product ion peptide fragment (e.g. y8, y10, b7, etc.).	String

Product Ion Formula	The formula of the product ion.	String
Product Neutral Formula	The formula of the product ion. This is deprecated, and "ProductIonFormula" should be used instead.	String
Product Adduct	The adduct applied to the product ion.	String
Fragment Ion Type	The type of the product ion (y, b, c, z, a, x, precursor)	IonType
Fragment Ion Ordinal	Position of the amino acid in the peptide after (C-terminal of) which the peptide was cleaved upon fragmentation. (e.g. 8, 10, 7, etc.)	Int32
Cleavage Aa	Specific amino acid residue in the peptide after (C-terminal of) which the peptide was cleaved upon fragmentation. (e.g. P, M, S, T, etc.)	Char
Loss Neutral Mass	The total mass of all neutral losses from this fragment.	Double
Losses	A comma separated list of all neutral losses from this fragment	String
Loss Formulas	A comma separated list of the chemical forumulas for all neutral losses from this fragment, or empty if not all losses have formulas	String
Quantitative	Whether the transition's peak area should be included when quantifying peptides.	Boolean
Explicit Collision Energy	The exact desired collision energy to be used in SRM methods or transitions lists for a target, overriding all model or optimization	Double

	library or per-precursor explicit values.	
Explicit SLens	The exact desired SLens value (Thermo instruments only) to be used in SRM methods or transitions lists for a target.	Double
Explicit Cone Voltage	The exact desired cone voltage (Waters instruments only) to be used in SRM methods or transitions lists for a target.	Double
Explicit Declustering Potential	The exact desired declustering potential (SCIEX instruments only) to be used in SRM methods or transitions lists for a target, overriding all model values.	Double
Explicit Ion Mobility High Energy Offset	The ion mobility high energy offset to be used when extracting chromatograms	Double
Transition Note	A free text note associated with the transition by clicking Edit Note on the Edit menu	String
Library Rank	The rank based on LibraryIntensity of this transition among all transitions allowed by the transition Filter settings, shown in the user interface as “(rank #)”.	Int32
Library Intensity	The MS/MS peak intensity corresponding to the transition product ion in the matching library spectrum.	Double
Isotope Dist Index	Zero for the monoisotopic peak, 1 for M+1, 2 for M+2, etc.	Int32
Isotope Dist Rank	The rank based on the IsotopeDistProportion among all isotope peaks for the predicted isotope distribution, shown in the user interface as “(irank #)”. Currently only available for precursor transitions filtered from high resolution MS1 scans.	Int32

Isotope Dist Proportion	The proportion of the entire isotope distribution predicted for this isotope peak. Currently only available for precursor transitions filtered from high resolution MS1 scans.	Double
Full Scan Filter Width	Full Scan Filter Width	Double
Transition Is Decoy	True if this is a decoy transition	Boolean
Product Decoy Mz Shift	Shift in m/z applied to the product ion to create the decoy m/z.	Int32
Transition Locator	Unique identifier of the transition within the document. This begins with "Transition:".	String

TransitionResultSummary

Name	Description	Type
Retention Time	Retention time at the maximum intensity for a transition peak.	RetentionTimeSummary

Name	Description	Type
Min Retention Time	Minimum of the transition RetentionTime values.	Double
Max Retention Time	Maximum of the transition RetentionTime values.	Double
Range Retention	The difference between MaxRetentionTime and MinRetentionTime, which can be used to gauge	Double

	Time	the spread of retention times measured.	
	Mean Retention Time	Mean of the transition RetentionTime values.	Double
	Stdev Retention Time	Standard deviation of the transition RetentionTime values.	Double
	Cv Retention Time	Coefficient of variation (CV) of the transition RetentionTime values.	Double
Fwhm	Full width at half max (FWHM) for the transition peak.	FwhmSummary	

Name	Description	Type
Mean Fwhm	Mean of the transition Fwhm (peak width) values.	Double
Stdev Fwhm	Standard deviation of the transition Fwhm (peak width) values.	Double
Cv Fwhm	Coefficient of variation (CV) of the transition Fwhm (peak width) values	Double

Area	Area under the curve (AUC), minus background, for the transition peak.	AreaSummary

Name	Description	Type
Mean Area	Mean of the transition Area values.	Double

	Stdev Area	Standard deviation of the transition Area values	Double
	Cv Area	Coefficient of variation (CV) of the transition Area values.	Double
Area Normalized	The Area normalized to the sum of the Area values for all transitions in the document.		AreaNormalizedSummary

Name	Description	Type
Mean Area Normalized	Mean of the transition AreaNormalized values	Double
Stdev Area Normalized	Standard deviation of the transition AreaNormalized values.	Double
Cv Area Normalized	Coefficient of variation (CV) of the transition AreaNormalized values.	Double

Area Ratio	The ratio of the Area of this transition to its corresponding transition in the first internal standard label type, before version 0.7 this was always light/heavy, and appeared on the heavy transitions.	AreaRatioSummary

Name	Description	Type
Mean Area Ratio	Mean of the transition AreaRatio values.	Double
Stdev Area Ratio	Standard deviation of the transition AreaRatio values.	Double
Cv Area Ratio	Coefficient of variation (CV) of the transition	Double

	AreaRatio values.

Precursor Result

Name	Description	Type
Precursor	Precursor	Precursor
Detection Q Value	A false discovery rate (FDR) score assigned to each chosen target peak after applying a mProphet model.	Double
Detection Z Score	A normalized mProphet score assigned to each chosen peak (target and decoy) after applying a mProphet model, expressed as the number of standard deviations (SD) from the mean decoy score.	Double
Precursor Peak Found Ratio	The ratio of transitions for which a peak was measured to the total number of transitions in the peptide. Peak indicators in the peptide tree view correspond to green = 1.0 (all transitions integrated), orange >= 0.5, red < 0.5.	Double
Best Retention Time	The RetentionTime value of the transition with the highest maximum intensity for the precursor.	Double
Max Fwhm	The maximum full width at half max (FWHM) of the transitions for the precursor.	Double
Min Start Time	Minimum StartTime of all transitions for a precursor. Unless manually edited all transitions for a precursor use the same integration boundaries	Double

Max End Time	Maximum EndTime of all transitions for a precursor. Unless manually edited all transitions for a precursor use the same integration boundaries.	Double
Total Area	The summed Area values of all individual transitions for the particular precursor.	Double
Total Area MS1	Total Area MS1	Double
Total Area Fragment	Total Area Fragment	Double
Total Background	The summed Background values of all individual transitions for the particular precursor	Double
Total Background MS1	Total Background MS1	Double
Total Background Fragment	Total Background Fragment	Double
Total Area Ratio	The ratio of the TotalArea of this precursor to the first internal standard label type, before version 0.7 this was always light/heavy, and appeared on the heavy precursor.	Double
Ratio Dot Product	Ratio Dot Product	Double
Total Area Normalized	The TotalArea normalized to the sum of the TotalArea values for all peptide precursors in the document	Double
Max Height	Max Height	Double

Average Mass Error PPM	Average Mass Error PPM	Double
Count Truncated	The number of transitions for a precursor that integrate a peak with a boundary at either end of the acquisition time range, where intensity at the end is greater than 1% of the entire peak height higher than the other extent.	Int32
Identified	True if a MS/MS peptide identification exists for the result file at a time between the peak integration boundaries.	PeakIdentification
Library Dot Product	The dot-product between the individual transition peak areas of the precursor and the intensities of the matching ion peaks in the matched MS/MS spectral library spectrum (Note: as of v1.4, this is now 1 – Arcos(dotp)/(Pi/2) where dotp is the value described above. a.k.a. Normalize Spectrum Contrast Angle), or #N/A if the precursor has not matching library spectrum or has fewer than 4 transitions. This is a 35 useful value for method refinement. It works best when 6 or more transitions are present.	Double
Isotope Dot Product	The dot-product calculation described above, but between the individual precursor (M, M+1, M+2, etc.) peak areas of the precursor and the intensities of the predicted isotope distribution, or #N/A if the transition is not a precursor isotope, or the chromatogram was not extracted from high resolution MS1 data.	Double
User Set Total	True if the default choice of peak or its boundaries was manually altered.	UserSet

Opt Step	Optimization step value indicating distance from the default value for the parameter being optimized, 0 for the default parameter value, or if no optimization is being performed in the replicate.	Int32
Opt Collision Energy	The collision energy value corresponding to the OptStep if collision energy optimization is being performed	Double
Opt Declustering Potential	The declustering potential value corresponding to the OptStep if declustering potential optimization is being performed	Double
Opt Compensation Voltage	The compensation voltage value (for ion mobility filtering) corresponding to the OptStep if compensation voltage optimization is being performed	Double
Collisional Cross Section	A measure of ion mobility, in square angstroms, which is typically converted to appropriate units (eg drift time, inverseK0) and used in extracting chromatograms from ion mobility mass spectra.	Double
Ion Mobility MS1	Center of the ion mobility filter window used in chromatogram extraction for a precursor ion.	Double
Ion Mobility Fragment	Center of the ion mobility filter window used in chromatogram extraction for a fragment ion. This may differ from the value for precursor ions , as fragment ions may move faster due to more energetic collisions,	Double
Ion Mobility Window	Width of the ion mobility filter window used in chromatogram extraction.	Double

Ion Mobility Units	Units for ion mobility used in chromatogram extraction.	String
Precursor Quantification	Values related to using the isotopolog response curve to quantify the precursor result.	PrecursorQuantificationResult
Precursor Replicate Note	A free text note associated with a result set of the precursor using the Results Grid.	String
Molecule Result	Molecule Result	Molecule Result
Precursor Result Locator	Unique identifier of the precursor result within the document. This begins with "PrecursorResult:" and usually ends with the replicate name but may have additional attributes for the optimization step and result file.	String

QuantificationResult

Name	Description	Type
Normalized Area	Value obtained by normalizing the peptide/molecule intensity according to either the explicit "Normalization Method" for the peptide/molecule or the normalization method specified on: Settings > Peptide Settings > Quantification	Double
Calculated Concentration	The concentration of the analyte is calculated by either: 1. Using the calibration curve (if the Peptide Settings > Quantification has a Regression Fit specified) 2. Using the ratio to internal standard (or surrogate) and multiplying by the Internal Standard Concentration	Double
Accuracy	Ratio of Calculated Concentration the Analyte Concentration (specified on the Replicate)	Double

Transition Result

Name	Description	Type
Transition	Transition	Transition
Retention Time	Retention time at the maximum intensity for a transition peak.	Double
Fwhm	Full width at half max (FWHM) for the transition peak.	Double
Fwhm Degenerate	Fwhm Degenerate	Boolean
Start Time	Retention time at the starting integration boundary for the transition peak	Double
End Time	Retention time at the ending integration boundary for the transition peak.	Double
Area	Area under the curve (AUC), minus background, for the transition peak.	Double
Background	The area of the rectangle formed by the integration boundaries, and the baseline and a line perpendicular to minimum intersection intensity between the integration boundaries and the chromatogram for the transition peak.	Double
Area Ratio	The ratio of the Area of this transition to its corresponding transition in the first internal standard label type, before version 0.7 this was always light/heavy, and appeared on the heavy transitions.	Double
Area Normalized	The Area normalized to the sum of the Area values for all transitions in the document.	Double
Height	The maximum intensity of the points between the transition peak integration boundaries.	Double
Mass Error PPM	Mass Error PPM	Double
Truncated	True if the integrated a peak has a boundary at either	Boolean

	end of the acquisition time range, where intensity at the end is greater than 1% of the entire peak height higher than the other extent.	
Peak Rank	The rank based on Area of this transition among all other transitions of the same precursor.	Int32
Peak Rank By Level	Peak area ranking in a specific replicate by MS level (i.e. MS1 and MS/MS get ranked separately)	Int32
User Set Peak	True if the default choice of peak or its boundaries was manually altered	UserSet
Opt Step	Optimization step value indicating distance from the default value for the parameter being optimized, 0 for the default parameter value, or if no optimization is being performed in the replicate.	Int32
Points Across Peak	Number of chromatogram points between the start and end time of the integrated peak.	Int32
Cycle Time Across Peak	Cycle time (in seconds) across the integrated peak.	Double
Skewness	A measure of the asymmetry of the chromatogram peak.	Double
Kurtosis	A measure of the "tailedness" of the chromatogram peak.	Double
Peak StdDev	The standard deviation of the chromatographic peak.	Double
Shape Correlation	The Pearson correlation of this transition's chromatographic peak compared to the median peak shape of all of the transitions under the same precursor.	Double
Coeluting	True if this transition's peak has similar apex and extents as the other transitions within the peak group.	Boolean
Ion Mobility	Center of the ion mobility filter window used in	Double

Fragment	chromatogram extraction for a fragment ion. This may differ from the value for precursor ions , as fragment ions may move faster due to more energetic collisions,	
Chromatogram	Chromatogram for the transition and replicate.	Chromatogram
Transition Replicate Note	A free text note associated with a result set of the transition using the Results Grid.	String
Transition Result Is Quantitative	Whether this result is treated as quantitative, based on the user-modifiable Quantitative property of the Transition and whether the MS/MS Full Scan Acquisition Method is DDA which treats all fragment ions as non-quantitative.	Boolean
Transition Result Is MS1	Whether this result was obtained from an MS1 scan.	Boolean
Precursor Result	Precursor Result	Precursor Result
Transition Result Locator	Unique identifier of the transition result within the document. This begins with "TransitionResult:" and usually ends with the replicate name, but may have additional attributes for the optimization step and result file.	String

PrecursorQuantificationResult

Name	Description	Type
Precursor Normalized Area	The normalized area of the Precursor Result. This is equal to the Total Area of the Precursor Result normalized according to the Normalization Method of the Peptide. If the Peptide Normalization Method is "None" or ratio to a label, then the Precursor Normalized Area will be equal to the Precursor Total Area.	Double

Precursor Calculated Concentration	The concentration of the Precursor Result calculated using the isotopolog response curve.	Double
Precursor Accuracy	Ratio of the Precursor Calculated Concentration to the Precursor Concentration specified on the Precursor.	Double
Qualitative Ion Ratio	Ratio of the sum of peak areas of the the non-quantitative transitions to the sum of the peak areas of the quantitative transitions under this molecule or peptide.	Double
Qualitative Ion Ratio Status	Description of how the Qualitative Ion Ratio compares to the Target Qualitative Ion Ratio. If the Qualitative Ion Ratio Threshold has been specified in the Quantification Settings, then Qualitative Ion Ratio Status will be either "pass" or "fail". If the Qualitative Ion Ratio Threshold has not been specified then Qualitative Ion Ratio Status will be either "equal", "low", or "high", depending on how it compares to the Target Qualitative Ion Ratio.	ValueStatus
Batch Target Qualitative Ion Ratio	Target Qualitative Ion Ratio calculated using the subset of external standard replicates that have the same Batch Name as this replicate.	Double

Chromatogram

Name	Description	Type
Chromatogram Precursor M/Z	Precursor m/z of the chromatogram	Double
Chromatogram Product M/Z	Product m/z of the chromatogram	Double
Chromatogram Extraction Width	Full width of the channel over which the spectrum intensities were summed	Double
Chromatogram Start Time	First retention time in the chromatogram	Double

Chromatogram End Time	Last retention time in the chromatogram	Double
Chromatogram Ion Mobility	Center of the ion mobility window that was used to filter spectra during chromatogram extraction	Double
Chromatogram Ion Mobility Extraction Width	Full width of the ion mobility window that was used to filter spectra during chromatogram extraction	Double
Chromatogram Ion Mobility Units	Units of the chromatogram ion mobility and chromatogram ion mobility extraction width	String
Chromatogram Source	Type of scans from which the chromatogram was extracted: one of "fragment", "sim", "ms1", or "unknown"	ChromSource
Raw Data	The raw (uninterpolated) chromatogram data. The chromatograms have unevenly spaced times, and the chromatograms of each transition potentially has a different number of points.	Data

Name	Description	Type
Raw Number of Points	The number of points in the raw (uninterpolated) chromatogram.	Int32
Raw Times	The retention times in the raw (uninterpolated) chromatogram.	FormattableList`1
Raw Intensities	The intensities of the raw (uninterpolated) chromatogram.	FormattableList`1
Raw Mass Errors	The mass errors of the raw (uninterpolated) chromatogram.	FormattableList`1
Raw Spectrum	Identifiers of the spectra that contributed to the points in the	FormattableList`1

	Ids	raw (uninterpolated) chromatogram.	
Interpolated Data	Chromatogram data which was interpolated in the time dimension so that the retention times are evenly spaced, and all transitions within the peptide or molecule have the same number of points.		Data

Name	Description	Type
Interpolated Number of Points	The number of points in the interpolated chromatogram.	Int32
Interpolated Times	The retention times in the interpolated chromatogram.	FormattableList`1
Interpolated Intensities	Chromatogram intensities from the interpolated data.	FormattableList`1
Interpolated Mass Errors	Chromatogram mass errors from the interpolated data.	FormattableList`1
Interpolated Spectrum Ids	Identifiers of the spectra that contributed to the points in the interpolated chromatogram.	FormattableList`1