

Summary

The summary file contains summary information for all the raw files processed with a single MaxQuant run. The summary information consists of some MaxQuant parameters, information of the raw file contents, and statistics on the peak detection. Based on this file a quick overview can be gathered on the quality of the data in the raw file.

The last row in this file contains the summary information for each column on each of the processed files.

Name	Separator	Description
Raw file		The raw file processed.
Experiment		Experiment name assigned to this LC-MS run in the experimental design.
Fraction		Fraction assigned to this LC-MS run in the experimental design.
Enzyme		The protease used to digest the protein sample.
Enzyme mode		The protease used to digest the protein sample.
Enzyme first search		The protease used for the first search.
Enzyme mode first search		The protease used for the first search.
Use enzyme first search		Marked with '+' when a different protease setup was used for the first search.
Variable modifications		The variable modification(s) used during the identification of peptides.
Fixed modifications		The fixed modification(s) used during the identification of peptides.
Multi modifications		The multi modification(s) used during the identification of peptides.
Variable modifications first search		The variable modification(s) used during the first search.
Use variable modifications first search		Marked with '+' when different variable modifications were used for the first search.
Requantify		The number of labels used.
Multiplicity		The number of labels used.
Max. missed cleavages		The maximum allowed number of missed cleavages.
Labels0		The labels used in the labeling experiment. Allowed values for X: 0=light; 1=medium; 2=heavy label partner.
LC-MS run type		The type of LC-MS run. Usually it will be 'Standard' which refers to a conventional shotgun proteomics run with data-dependent MS/MS.
Time-dependent recalibration		When marked with '+', time-dependent recalibration was applied to improve the data quality.
MS		The number of MS spectra recorded in this raw file.
MS/MS		The number of MS/MS spectra recorded in this raw file.
MS3		The number of MS3 spectra recorded in this raw file.
MS/MS Submitted		The number of tandem MS spectra submitted for analysis.
MS/MS Submitted (SIL)		The number of tandem MS spectra submitted for analysis, where the precursor ion was detected as part of a labeling cluster.
MS/MS Submitted (ISO)		The number of tandem MS spectra submitted for analysis, where the precursor ion was detected as an isotopic pattern.
MS/MS Submitted (PEAK)		The number of tandem MS spectra submitted for analysis, where the precursor ion was detected as a single peak.
MS/MS Identified		The total number of identified tandem MS spectra.
MS/MS Identified (SIL)		The total number of identified tandem MS spectra, where the precursor ion was detected as part of a labeling cluster.
MS/MS Identified (ISO)		The total number of identified tandem MS spectra, where the precursor ion was detected as an isotopic pattern.
MS/MS Identified (PEAK)		The total number of identified tandem MS spectra, where the precursor ion was detected as a single peak.
MS/MS Identified [%]		The percentage of identified tandem MS spectra.
MS/MS Identified (SIL) [%]		The percentage of identified tandem MS spectra, where the precursor ion was detected as part of a labeling cluster.
MS/MS Identified (ISO) [%]		The percentage of identified tandem MS spectra, where the precursor ion was detected as an isotopic pattern.
MS/MS Identified (PEAK) [%]		The percentage of identified tandem MS spectra, where the precursor ion was detected as a single peak.
Peptide Sequences Identified		The total number of unique peptide amino acid sequences identified from the recorded tandem mass spectra.

Peaks		The total number of peaks detected in the full scans.
Peaks Sequenced		The total number of peaks sequenced by tandem MS.
Peaks Sequenced [%]		The percentage of peaks sequenced by tandem MS.
Peaks Repeatedly Sequenced		The total number of peaks repeatedly sequenced (i.e. 1 or more times) by tandem MS.
Peaks Repeatedly Sequenced [%]		The percentage of peaks repeatedly sequenced (i.e. 1 or more times) by tandem MS.
Isotope Patterns		The total number of detected isotope patterns.
Isotope Patterns Sequenced		The total number of isotope patterns sequenced by tandem MS.
Isotope Patterns Sequenced (z>1)		The total number of isotope patterns sequenced by tandem MS with a charge state of 2 or more.
Isotope Patterns Sequenced [%]		The percentage of isotope patterns sequenced by tandem MS.
Isotope Patterns Sequenced (z>1) [%]		The percentage of isotope patterns sequenced by tandem MS with a charge state of 2 or more.
Isotope Patterns Repeatedly Sequenced		The total number of isotope patterns repeatedly sequenced (i.e. 1 or more times) by tandem MS.
Isotope Patterns Repeatedly Sequenced [%]		The percentage of isotope patterns repeatedly sequenced (i.e. 1 or more times) by tandem MS.
Recalibrated		When marked with '+', the masses taken from the raw file were recalibrated.
Av. Absolute Mass Deviation [ppm]		The average absolute mass deviation found comparing to the identification mass in parts per million.
Mass Standard Deviation [ppm]		The standard deviation of the mass deviation found comparing to the identification mass in parts per million.
Av. Absolute Mass Deviation [mDa]		The average absolute mass deviation found comparing to the identification mass in milli-Dalton.
Mass Standard Deviation [mDa]		The standard deviation of the mass deviation found comparing to the identification mass in milli-Dalton.
Label free norm param		The normalization factor used to scale the intensity values in a label-free experiment.

Evidence

The evidence file combines all the information about the identified peptides and normally is the only file required for processing the results. Additional information about the peptides, modifications, proteins, etc. can be found in the other files by unique identifier linkage.

Name	Separator	Description
Sequence		The identified AA sequence of the peptide.
Length		The length of the sequence stored in the column 'Sequence'.
Modifications		Post-translational modifications contained within the identified peptide sequence.
Modified sequence		Sequence representation including the post-translational modifications (abbreviation of the modification in brackets before the modified AA). The sequence is always surrounded by underscore characters ('_').
Deamidation (NQ) Probabilities		Sequence representation of the peptide including PTM positioning probabilities ([0..1], where 1 is best match) for 'Deamidation (NQ)'.
Oxidation (M) Probabilities		Sequence representation of the peptide including PTM positioning probabilities ([0..1], where 1 is best match) for 'Oxidation (M)'.
Deamidation (NQ) Score Diffs		Sequence representation for each of the possible PTM positions in each possible configuration, the difference is calculated between the identification score with the PTM added to that position and the best scoring identification where no PTM is added to that position. When this value is negative, it is unlikely that the particular modification is located at this position.
Oxidation (M) Score Diffs		Sequence representation for each of the possible PTM positions in each possible configuration, the difference is calculated between the identification score with the PTM added to that position and the best scoring identification where no PTM is added to that position. When this value is negative, it is unlikely that the particular modification is located at this position.
Acetyl (Protein N-term)		The number of occurrences of the modification 'Acetyl (Protein N-term)'.
Deamidation (NQ)		The number of occurrences of the modification 'Deamidation (NQ)'.
Oxidation (M)		The number of occurrences of the modification 'Oxidation (M)'.
Missed cleavages		Number of missed enzymatic cleavages.
Proteins		The identifiers of the proteins this particular peptide is associated with.
Leading proteins		The identifiers of the proteins in the proteinGroups file, with this protein as best match, this particular peptide is associated with. When multiple matches are found here, the best scoring protein can be found in the 'Leading Razor Protein' column.
Leading razor protein		The identifier of the best scoring protein, from the proteinGroups file this, this peptide is associated to.
Type		The type of the feature. 'MSMS' for an MS/MS spectrum without an MS1 isotope pattern assigned. 'ISO-MSMS' MS1 isotope cluster identified by MS/MS. 'MULTI-MSMS' MS1 labeling cluster identified by MS/MS. 'MULTI-SECPEP' MS1 labeling cluster identified by MS/MS as second peptide. 'MULTI-MATCH' MS1 labeling cluster identified by matching between runs. In case of label-free data there is no difference between 'MULTI' and 'ISO'.
Raw file		The name of the RAW-file the mass spectral data was derived from.
Fraction		The fraction in which this peptide was detected.
Experiment		
MS/MS m/z		The m/z used for fragmentation (not necessarily the mono-isotopic m/z).
Charge		The charge-state of the precursor ion.
m/z		The recalibrated mass-over-charge value of the precursor ion.
Mass		The predicted monoisotopic mass of the identified peptide sequence.
Resolution		The resolution of precursor ion measured in Full Width at Half Maximum (FWHM).
Uncalibrated - Calibrated m/z [ppm]		The difference between the uncalibrated and recalibrated mass-over-charge value of the precursor ion measured in parts-per-million. This gives an indication of the mass drift in the original data, which was automatically corrected by MaxQuant.

Uncalibrated - Calibrated m/z [Da]		The difference between the uncalibrated and recalibrated mass-over-charge value of the precursor ion measured in parts-per-million. This gives an indication of the mass drift in the original data, which was automatically corrected by MaxQuant.
Mass error [ppm]		Mass error of the recalibrated mass-over-charge value of the precursor ion in comparison to the predicted monoisotopic mass of the identified peptide sequence in parts per million.
Mass error [Da]		Mass error of the recalibrated mass-over-charge value of the precursor ion in comparison to the predicted monoisotopic mass of the identified peptide sequence in milli-Dalton.
Uncalibrated mass error [ppm]		Mass error of the uncalibrated mass-over-charge value of the precursor ion in comparison to the predicted monoisotopic mass of the identified peptide sequence. Note: This column can contain missing values (denoted as NaN).
Uncalibrated mass error [Da]		Mass error of the uncalibrated mass-over-charge value of the precursor ion in comparison to the predicted monoisotopic mass of the identified peptide sequence. Note: This column can contain missing values (denoted as NaN).
Max intensity m/z 0		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Retention time		The uncalibrated retention time in minutes in the elution profile of the precursor ion.
Retention length		The total retention time length of the peak (last time point - first time point).
Calibrated retention time		The recalibrated retention time in minutes in the elution profile of the precursor ion.
Calibrated retention time start		The recalibrated retention start in minutes in the elution profile of the precursor ion.
Calibrated retention time finish		The recalibrated retention finish in minutes in the elution profile of the precursor ion.
Retention time calibration		The difference in minutes between the uncalibrated and recalibrated retention time. This gives an indication of the retention time drift in the original data, which was automatically corrected by MaxQuant. Note: This column can contain missing values (NaN).
Match time difference		When the option match between runs is used in MaxQuant, this value indicates the time difference between the feature from the raw file it was taken from and the feature from the raw file it was matched to.
Match m/z difference		When the option match between runs is used in MaxQuant, this value indicates the m/z difference between the feature from the raw file it was taken from and the feature from the raw file it was matched to.
Match q-value		This is the q-value for features that have been identified by 'matching between runs'.
Match score		The andromeda score of the MS/MS identification that is the source of this identification by 'matching between runs'.
Number of data points		The number of data points (peak centroids) collected for this peptide feature.
Number of scans		The number of MS scans that the 3d peaks of this peptide feature are overlapping with.
Number of isotopic peaks		The number of isotopic peaks contained in this peptide feature.
PIF		Short for Parent Ion Fraction; indicates the fraction the target peak makes up of the total intensity in the inclusion window.
Fraction of total spectrum		The percentage the ion intensity makes up of the total intensity of the whole spectrum.
Base peak fraction		The percentage the parent ion intensity in comparison to the highest peak in the MS spectrum.
PEP		Posterior Error Probability of the identification. This value essentially operates as a p-value, where smaller is more significant.
MS/MS count		The number of sequencing events for this sequence, which matches the number of identifiers stored in the column MS/MS IDs.
MS/MS scan number		The RAW-file derived scan number of the MS/MS with the highest peptide identification score (the highest score is stored in the column 'Score').
Score		Andromeda score for the best associated MS/MS spectrum.
Delta score		Score difference to the second best identified peptide.
Combinatorics		Number of possible distributions of the modifications over the peptide sequence.

Intensity		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Reporter PIF		
Reporter fraction		
Reverse		When marked with '+', this particular peptide was found to be part of a protein derived from the reversed part of the decoy database. These should be removed for further data analysis.
Potential contaminant		When marked with '+', this particular peptide was found to be part of a commonly occurring contaminant. These should be removed for further data analysis.
id		A unique (consecutive) identifier for each row in the evidence table, which is used to cross-link the information in this file with the information stored in the other files.
Protein group IDs		The identifier of the protein-group this redundant peptide sequence is associated with, which can be used to look up the extended protein information in the file 'proteinGroups.txt'. As a single peptide can be linked to multiple proteins (e.g. in the case of razor-proteins), multiple ids can be stored here separated by a semicolon. As a protein can be identified by multiple peptides, the same id can be found in different rows.
Peptide ID		The identifier of the non-redundant peptide sequence.
Mod. peptide ID		Identifier of the associated modification summary stored in the file 'modificationSpecificPeptides.txt'.
MS/MS IDs		Identifier(s) of the associated MS/MS summary(s) stored in the file 'msms.txt'.
Best MS/MS		Identifier(s) of the best MS/MS associated spectrum stored in the file 'msms.txt'.
Deamidation (NQ) site IDs		Identifier(s) of the modification summary stored in the file 'Deamidation (NQ)Sites.txt'.
Oxidation (M) site IDs		Identifier(s) of the modification summary stored in the file 'Oxidation (M)Sites.txt'.

Peptides

The peptides table contains information on the identified peptides in the processed raw-files.

Name	Separator	Description
Sequence		The amino acid sequence of the identified peptide.
N-term cleavage window		Sequence window from -15 to 15 around the N-terminal cleavage site of this peptide.
C-term cleavage window		Sequence window from -15 to 15 around the C-terminal cleavage site of this peptide.
Amino acid before		The amino acid in the protein sequence before the peptide.
First amino acid		The amino acid in the first position of the peptide sequence.
Second amino acid		The amino acid in the first position of the peptide sequence.
Second last amino acid		The amino acid in the last position of the peptide sequence.
Last amino acid		The amino acid in the last position of the peptide sequence.
Amino acid after		The amino acid in the protein sequence after the peptide.
A Count		The number of instances of the 'A' amino acid contained within the sequence.
R Count		The number of instances of the 'R' amino acid contained within the sequence.
N Count		The number of instances of the 'N' amino acid contained within the sequence.
D Count		The number of instances of the 'D' amino acid contained within the sequence.
C Count		The number of instances of the 'C' amino acid contained within the sequence.
Q Count		The number of instances of the 'Q' amino acid contained within the sequence.
E Count		The number of instances of the 'E' amino acid contained within the sequence.
G Count		The number of instances of the 'G' amino acid contained within the sequence.
H Count		The number of instances of the 'H' amino acid contained within the sequence.
I Count		The number of instances of the 'I' amino acid contained within the sequence.
L Count		The number of instances of the 'L' amino acid contained within the sequence.
K Count		The number of instances of the 'K' amino acid contained within the sequence.
M Count		The number of instances of the 'M' amino acid contained within the sequence.
F Count		The number of instances of the 'F' amino acid contained within the sequence.
P Count		The number of instances of the 'P' amino acid contained within the sequence.
S Count		The number of instances of the 'S' amino acid contained within the sequence.
T Count		The number of instances of the 'T' amino acid contained within the sequence.
W Count		The number of instances of the 'W' amino acid contained within the sequence.
Y Count		The number of instances of the 'Y' amino acid contained within the sequence.
V Count		The number of instances of the 'V' amino acid contained within the sequence.
U Count		The number of instances of the 'U' amino acid contained within the sequence.
O Count		The number of instances of the 'O' amino acid contained within the sequence.
Length		The length of the sequence stored in the column "Sequence".
Missed cleavages		Number of missed enzymatic cleavages.
Mass		Monoisotopic mass of the peptide.
Proteins		Identifiers of proteins this peptide is associated with.
Leading razor protein		Identifier of the leading protein in the protein group which uses this peptide for quantification. (Either unique or razor.)
Start position		Position of the first amino acid of this peptide in the protein sequence. (one-based)
End position		Position of the last amino acid of this peptide in the protein sequence. (one-based)

Unique (Groups)		When marked with '+', this particular peptide is unique to a single protein group in the proteinGroups file.
Unique (Proteins)		When marked with '+', this particular peptide is unique to a single protein sequence in the fasta file(s).
Charges		All charge states that have been observed.
PEP		Posterior Error Probability of the identification. This value essentially operates as a p-value, where smaller is more significant.
Score		Highest Andromeda score for the associated MS/MS spectra.
Identification type SER1		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER10		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER100		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER101		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER102		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER103		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER104		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER105		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER106		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER108		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER109		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER11		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER12		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER13		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER133		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER134		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER135		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER136		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER137		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER138		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER139		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER14		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER140		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER141		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER142		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER143		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER144		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER145		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER146		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER147		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER148		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER149		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER15		Indicates whether this experiment was identified by MS/MS or only by matching between runs.

Intensity SER86		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER87		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER88		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER89		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER9		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER91		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER92		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER94		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER95		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER96		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER97		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER98		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER99		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Reverse		When marked with '+', this particular peptide was found to be part of a protein derived from the reversed part of the decoy database. These should be removed for further data analysis.
Potential contaminant		When marked with '+', this particular peptide was found to be part of a commonly occurring contaminant. These should be removed for further data analysis.
id		A unique (consecutive) identifier for each row in the peptides table, which is used to cross-link the information in this table with the information stored in the other tables.
Protein group IDs		The identifiers of the protein groups this peptide was linked to, referenced against the proteinGroups table.
Mod. peptide IDs		Identifier(s) for peptide sequence(s), associated with the peptide, referenced against the corresponding modified peptides table.
Evidence IDs		Identifier(s) for analyzed peptide evidence associated with the protein group referenced against the evidence table.
MS/MS IDs		The identifiers of the MS/MS scans identifying this peptide, referenced against the msms table.
Best MS/MS		The identifier of the best (in terms of quality) MS/MS scan identifying this peptide, referenced against the msms table.
Deamidation (NQ) site IDs		Identifier(s) for site(s) associated with the protein group, which show(s) evidence of the modification, referenced against the appropriate modification site file.
Oxidation (M) site IDs		Identifier(s) for site(s) associated with the protein group, which show(s) evidence of the modification, referenced against the appropriate modification site file.
MS/MS Count		
LFQ intensity SER105		
LFQ intensity SER106		
LFQ intensity SER108		

LFQ intensity SER109		
LFQ intensity SER11		
LFQ intensity SER12		
LFQ intensity SER13		
LFQ intensity SER14		
LFQ intensity SER143		
LFQ intensity SER144		
LFQ intensity SER145		
LFQ intensity SER146		
LFQ intensity SER147		
LFQ intensity SER15		
LFQ intensity SER156		
LFQ intensity SER157		
LFQ intensity SER170		
LFQ intensity SER171		
LFQ intensity SER172		
LFQ intensity SER183		
LFQ intensity SER184		
LFQ intensity SER185		
LFQ intensity SER186		
LFQ intensity SER187		
LFQ intensity SER26		
LFQ intensity SER27		
LFQ intensity SER28		
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LFQ intensity SER30		
LFQ intensity SER41		
LFQ intensity SER42		
LFQ intensity SER43		
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LFQ intensity SER56		
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LFQ intensity SER60		
LFQ intensity SER71		
LFQ intensity SER72		
LFQ intensity SER73		
LFQ intensity SER91		
LFQ intensity SER92		
LFQ intensity SER94		
LFQ intensity SER1		
LFQ intensity SER10		
LFQ intensity SER100		
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LFQ intensity SER104		
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LFQ intensity SER38		
LFQ intensity SER39		
LFQ intensity SER4		
LFQ intensity SER40		
LFQ intensity SER47		
LFQ intensity SER48		
LFQ intensity SER49		
LFQ intensity SER5		
LFQ intensity SER50		
LFQ intensity SER51		
LFQ intensity SER52		
LFQ intensity SER53		
LFQ intensity SER54		
LFQ intensity SER55		
LFQ intensity SER6		
LFQ intensity SER61		
LFQ intensity SER62		
LFQ intensity SER63		
LFQ intensity SER64		
LFQ intensity SER65		
LFQ intensity SER66		
LFQ intensity SER67		
LFQ intensity SER68		
LFQ intensity SER69		
LFQ intensity SER7		
LFQ intensity SER70		
LFQ intensity SER8		
LFQ intensity SER80		
LFQ intensity SER81		
LFQ intensity SER82		
LFQ intensity SER83		
LFQ intensity SER84		
LFQ intensity SER85		
LFQ intensity SER86		
LFQ intensity SER87		
LFQ intensity SER88		

LFQ intensity SER89		
LFQ intensity SER9		
LFQ intensity SER95		
LFQ intensity SER96		
LFQ intensity SER97		
LFQ intensity SER98		
LFQ intensity SER99		

Modification-specific peptides

Name	Separator	Description
Sequence		The identified AA sequence of the peptide.
Modifications		Post-translational modifications contained within the sequence. When no modifications exist, this is set to 'unmodified'.
Mass		Charge corrected mass of the precursor ion.
Mass Fractional Part		The values after the decimal point (ie value - floor(value)).
Protein Groups		IDs of the protein groups to which this peptide belongs.
Proteins		The identifiers of the proteins this particular peptide is associated with.
Unique (Groups)		When marked with '+', this particular peptide is unique to a single protein group in the proteinGroups file.
Unique (Proteins)		When marked with '+', this particular peptide is unique to a single protein sequence in the fasta file(s).
Acetyl (Protein N-term)		Number of Acetyl (Protein N-term) on this peptide.
Deamidation (NQ)		Number of Deamidation (NQ) on this peptide.
Oxidation (M)		Number of Oxidation (M) on this peptide.
Missed cleavages		Number of missed enzymatic cleavages.
Identification type SER1		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER10		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER100		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER101		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER102		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER103		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER104		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER105		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER106		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER108		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER109		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER11		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER12		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER13		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER133		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER134		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER135		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER136		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER137		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER138		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER139		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER14		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER140		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER141		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER142		Indicates whether this experiment was identified by MS/MS or only by matching between runs.

Experiment SER85		Number of evidence entries for this 'Experiment'.
Experiment SER86		Number of evidence entries for this 'Experiment'.
Experiment SER87		Number of evidence entries for this 'Experiment'.
Experiment SER88		Number of evidence entries for this 'Experiment'.
Experiment SER89		Number of evidence entries for this 'Experiment'.
Experiment SER9		Number of evidence entries for this 'Experiment'.
Experiment SER91		Number of evidence entries for this 'Experiment'.
Experiment SER92		Number of evidence entries for this 'Experiment'.
Experiment SER94		Number of evidence entries for this 'Experiment'.
Experiment SER95		Number of evidence entries for this 'Experiment'.
Experiment SER96		Number of evidence entries for this 'Experiment'.
Experiment SER97		Number of evidence entries for this 'Experiment'.
Experiment SER98		Number of evidence entries for this 'Experiment'.
Experiment SER99		Number of evidence entries for this 'Experiment'.
Retention time		Retention time in minutes averaged over the evidence entries belonging to this modification-specific peptide.
Calibrated retention time		Calibrated retention time averaged over the evidence entries belonging to this modification-specific peptide. Obviously this only makes sense if retention time recalibration has been performed which is the case when matching between run is selected.
Charges		All charge states that have been observed.
PEP		Posterior Error Probability of the identification. This value essentially operates as a p-value, where smaller is more significant.
MS/MS scan number		The RAW-file derived scan number of the MS/MS with the highest peptide identification score (the highest score is stored in the column 'Score').
Raw file		The name of the RAW-file the mass spectral data was derived from.
Score		Andromeda score for the best identified among the associated MS/MS spectra.
Delta score		Score difference to the second best identified peptide.
Reverse		When marked with '+', this particular peptide was found to be part of a protein derived from the reversed part of the decoy database. These should be removed for further data analysis.
Potential contaminant		When marked with '+', this particular peptide was found to be part of a commonly occurring contaminant. These should be removed for further data analysis.
Intensity		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER1		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER10		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER100		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER101		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER102		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER103		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER104		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER105		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER106		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.

Intensity SER97		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER98		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER99		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
id		A unique (consecutive) identifier for each row in the peptides table, which is used to cross-link the information in this table with the information stored in the other tables.
Protein group IDs		The identifiers of the protein groups this peptide was linked to, referenced against the proteinGroups table.
Peptide ID		Identifier of the associated peptide sequence summary, which can be found in the file 'peptides.txt'.
Evidence IDs		Identifier(s) for analyzed peptide evidence associated with the protein group referenced against the evidence table.
MS/MS IDs		The identifiers of the MS/MS scans identifying this peptide, referenced against the msms table.
Best MS/MS		The identifier of the best (in terms of quality) MS/MS scan identifying this peptide, referenced against the msms table.
Deamidation (NQ) site IDs		Identifier(s) for site(s) associated with this peptide, which show(s) evidence of the modification, referenced against the appropriate modification site file.
Oxidation (M) site IDs		Identifier(s) for site(s) associated with this peptide, which show(s) evidence of the modification, referenced against the appropriate modification site file.
MS/MS Count		

Deamidation (NQ) Sites

Name	Separator	Description
Proteins		Identifiers of proteins this site is associated with.
Positions within proteins		For each protein identifier in the 'Proteins' column you find here the position of the site in the respective protein sequence. The index of the first amino acid in the sequence is 1.
Leading proteins		
Protein		Identifier of the protein this peptide is associated with.
Fasta headers		Descriptions of proteins this peptide is associated with.
Localization prob		
Score diff		
PEP		The posterior error probability (PEP) of the best identified modified peptide containing this site.
Score		The Andromeda score of the best identified modified peptide containing this site.
Delta score		The Andromeda delta score of the best identified modified peptide containing this site.
Score for localization		The Andromeda score of the MS/MS spectrum used for calculating the localization score for this site.
Localization prob SER1		
Score diff SER1		
PEP SER1		
Score SER1		
Localization prob SER10		
Score diff SER10		
PEP SER10		
Score SER10		
Localization prob SER100		
Score diff SER100		
PEP SER100		
Score SER100		
Localization prob SER101		
Score diff SER101		
PEP SER101		
Score SER101		
Localization prob SER102		
Score diff SER102		
PEP SER102		
Score SER102		
Localization prob SER103		
Score diff SER103		
PEP SER103		
Score SER103		
Localization prob SER104		
Score diff SER104		
PEP SER104		
Score SER104		
Localization prob SER105		
Score diff SER105		
PEP SER105		
Score SER105		
Localization prob SER106		
Score diff SER106		
PEP SER106		
Score SER106		
Localization prob SER108		
Score diff SER108		
PEP SER108		
Score SER108		
Localization prob SER109		
Score diff SER109		

PEP SER109		
Score SER109		
Localization prob SER11		
Score diff SER11		
PEP SER11		
Score SER11		
Localization prob SER12		
Score diff SER12		
PEP SER12		
Score SER12		
Localization prob SER13		
Score diff SER13		
PEP SER13		
Score SER13		
Localization prob SER133		
Score diff SER133		
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Localization prob SER134		
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Localization prob SER14		
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Localization prob SER140		
Score diff SER140		
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Localization prob SER141		
Score diff SER141		
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Localization prob SER142		
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Localization prob SER143		
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Localization prob SER144		
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Localization prob SER145		
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Localization prob SER146		
Score diff SER146		
PEP SER146		
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Localization prob SER147		
Score diff SER147		
PEP SER147		
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Localization prob SER148		
Score diff SER148		
PEP SER148		
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Localization prob SER149		
Score diff SER149		
PEP SER149		
Score SER149		
Localization prob SER15		
Score diff SER15		
PEP SER15		
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Localization prob SER150		
Score diff SER150		
PEP SER150		
Score SER150		
Localization prob SER151		
Score diff SER151		
PEP SER151		
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Localization prob SER156		
Score diff SER156		
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Localization prob SER157		
Score diff SER157		
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Localization prob SER160		
Score diff SER160		
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Localization prob SER161		
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Localization prob SER162		
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Localization prob SER163		
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Localization prob SER164		
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Localization prob SER165		
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Localization prob SER17		
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Localization prob SER170		
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Localization prob SER171		
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Localization prob SER172		
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Localization prob SER175		
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Localization prob SER176		
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Localization prob SER18		
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Localization prob SER180		
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Localization prob SER181		
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Localization prob SER182		
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Localization prob SER183		
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Localization prob SER187		
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Score SER187		
Localization prob SER19		
Score diff SER19		
PEP SER19		
Score SER19		
Localization prob SER2		
Score diff SER2		
PEP SER2		
Score SER2		
Localization prob SER20		
Score diff SER20		
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Localization prob SER21		
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Localization prob SER27		
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Localization prob SER28		
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Localization prob SER29		
Score diff SER29		
PEP SER29		
Score SER29		
Localization prob SER3		
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Localization prob SER30		
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Localization prob SER32		
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Localization prob SER38		
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Localization prob SER4		
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Localization prob SER40		
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Localization prob SER41		
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Localization prob SER51		
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Localization prob SER7		
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Localization prob SER70		
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Localization prob SER73		
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Localization prob SER8		
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Localization prob SER80		
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Localization prob SER91		
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Localization prob SER92		
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Localization prob SER94		
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Localization prob SER97		
Score diff SER97		
PEP SER97		
Score SER97		
Localization prob SER98		
Score diff SER98		
PEP SER98		
Score SER98		
Localization prob SER99		
Score diff SER99		
PEP SER99		
Score SER99		
Diagnostic peak		

Number of Deamidation (NQ)		Different numbers of Deamidation (NQ) on peptides that this site is involved in.
Amino acid		
Sequence window		
Modification window		
Peptide window coverage		
Deamidation (NQ) Probabilities		
Deamidation (NQ) Score diffs		
Position in peptide		
Charge		Charge state of the precursor ion.
Mass error [ppm]		Mass error of the recalibrated mass-over-charge value of the precursor ion in comparison to the predicted monoisotopic mass of the identified peptide sequence.
Identification type SER1		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER10		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER100		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER101		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER102		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER103		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER104		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER105		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER106		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER108		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER109		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER11		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER12		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER13		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER133		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER134		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER135		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER136		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER137		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER138		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER139		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER14		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER140		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER141		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER142		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER143		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER144		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER145		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER146		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER147		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER148		Indicates whether this experiment was identified by MS/MS or only by matching between runs.

Intensity SER87		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER88		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER89		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER9		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER91		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER92		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER94		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER95		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER96		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER97		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER98		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER99		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Ratio mod/base SER1		
Ratio mod/base SER10		
Ratio mod/base SER100		
Ratio mod/base SER101		
Ratio mod/base SER102		
Ratio mod/base SER103		
Ratio mod/base SER104		
Ratio mod/base SER105		
Ratio mod/base SER106		
Ratio mod/base SER108		
Ratio mod/base SER109		
Ratio mod/base SER11		
Ratio mod/base SER12		
Ratio mod/base SER13		
Ratio mod/base SER133		
Ratio mod/base SER134		
Ratio mod/base SER135		
Ratio mod/base SER136		
Ratio mod/base SER137		
Ratio mod/base SER138		
Ratio mod/base SER139		
Ratio mod/base SER14		
Ratio mod/base SER140		
Ratio mod/base SER141		
Ratio mod/base SER142		
Ratio mod/base SER143		
Ratio mod/base SER144		
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Ratio mod/base SER9		
Ratio mod/base SER91		
Ratio mod/base SER92		
Ratio mod/base SER94		
Ratio mod/base SER95		
Ratio mod/base SER96		
Ratio mod/base SER97		
Ratio mod/base SER98		
Ratio mod/base SER99		
Intensity SER1___1		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER1___2		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER1___3		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER10___1		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER10___2		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER10___3		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.

Intensity SER97___1		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER97___2		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER97___3		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER98___1		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER98___2		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER98___3		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER99___1		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER99___2		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER99___3		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
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Occupancy ratioSER1		
Occupancy error scale SER1		
Occupancy SER10		
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Occupancy SER100		
Occupancy ratioSER100		
Occupancy error scale SER100		
Occupancy SER101		
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Occupancy error scale SER101		
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Occupancy error scale SER102		
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Occupancy ratioSER99		
Occupancy error scale SER99		
Reverse		When marked with '+', this particular peptide was found to be part of a protein derived from the reversed part of the protein sequence database. These should be removed for further data analysis.
Potential contaminant		When marked with '+', this particular peptide was found to be part of a commonly occurring contaminant. These should be removed for further data analysis.

id		A unique (consecutive) identifier for each row in the site table, which is used to cross-link the information in this file with the information stored in the other files.
Protein group IDs		The identifier of the protein-group this peptide sequence is associated with, which can be used to look up the extended protein information in the file 'proteinGroups.txt'. As a single peptide can be linked to multiple proteins (e.g. in the case of razor-proteins), multiple id's can be stored here separated by a semicolon. As a protein can be identified by multiple peptides, the same id can be found in different rows.
Positions		The positions of the modifications in the protein amino acid sequence.
Position		The position of the modification in the protein amino acid sequence.
Peptide IDs		Identifier(s) of the associated peptide sequence(s) summary, which can be found in the file 'peptides.txt'.
Mod. peptide IDs		Identifier(s) of the associated peptide sequence(s) summary, which can be found in the file 'modificationSpecificPeptides.txt'.
Evidence IDs		Identifier(s) for analyzed peptide evidence associated with the protein group referenced against the evidence table.
MS/MS IDs		The identifiers of the MS/MS scans identifying this peptide, referenced against the msms table.
Best localization evidence ID		
Best localization MS/MS ID		
Best localization raw file		
Best localization scan number		
Best score evidence ID		
Best score MS/MS ID		
Best score raw file		
Best score scan number		
Best PEP evidence ID		
Best PEP MS/MS ID		
Best PEP raw file		
Best PEP scan number		

Oxidation (M) Sites

Name	Separator	Description
Proteins		Identifiers of proteins this site is associated with.
Positions within proteins		For each protein identifier in the 'Proteins' column you find here the position of the site in the respective protein sequence. The index of the first amino acid in the sequence is 1.
Leading proteins		
Protein		Identifier of the protein this peptide is associated with.
Fasta headers		Descriptions of proteins this peptide is associated with.
Localization prob		
Score diff		
PEP		The posterior error probability (PEP) of the best identified modified peptide containing this site.
Score		The Andromeda score of the best identified modified peptide containing this site.
Delta score		The Andromeda delta score of the best identified modified peptide containing this site.
Score for localization		The Andromeda score of the MS/MS spectrum used for calculating the localization score for this site.
Localization prob SER1		
Score diff SER1		
PEP SER1		
Score SER1		
Localization prob SER10		
Score diff SER10		
PEP SER10		
Score SER10		
Localization prob SER100		
Score diff SER100		
PEP SER100		
Score SER100		
Localization prob SER101		
Score diff SER101		
PEP SER101		
Score SER101		
Localization prob SER102		
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Localization prob SER103		
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Score diff SER2		
PEP SER2		
Score SER2		
Localization prob SER20		
Score diff SER20		
PEP SER20		
Score SER20		
Localization prob SER21		
Score diff SER21		
PEP SER21		
Score SER21		
Localization prob SER23		
Score diff SER23		
PEP SER23		
Score SER23		
Localization prob SER24		
Score diff SER24		
PEP SER24		
Score SER24		
Localization prob SER25		
Score diff SER25		
PEP SER25		
Score SER25		
Localization prob SER26		
Score diff SER26		
PEP SER26		
Score SER26		
Localization prob SER27		
Score diff SER27		
PEP SER27		
Score SER27		
Localization prob SER28		
Score diff SER28		
PEP SER28		
Score SER28		
Localization prob SER29		
Score diff SER29		
PEP SER29		
Score SER29		
Localization prob SER3		
Score diff SER3		
PEP SER3		
Score SER3		
Localization prob SER30		
Score diff SER30		
PEP SER30		
Score SER30		
Localization prob SER32		
Score diff SER32		

PEP SER32		
Score SER32		
Localization prob SER33		
Score diff SER33		
PEP SER33		
Score SER33		
Localization prob SER34		
Score diff SER34		
PEP SER34		
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Localization prob SER35		
Score diff SER35		
PEP SER35		
Score SER35		
Localization prob SER36		
Score diff SER36		
PEP SER36		
Score SER36		
Localization prob SER37		
Score diff SER37		
PEP SER37		
Score SER37		
Localization prob SER38		
Score diff SER38		
PEP SER38		
Score SER38		
Localization prob SER39		
Score diff SER39		
PEP SER39		
Score SER39		
Localization prob SER4		
Score diff SER4		
PEP SER4		
Score SER4		
Localization prob SER40		
Score diff SER40		
PEP SER40		
Score SER40		
Localization prob SER41		
Score diff SER41		
PEP SER41		
Score SER41		
Localization prob SER42		
Score diff SER42		
PEP SER42		
Score SER42		
Localization prob SER43		
Score diff SER43		
PEP SER43		
Score SER43		
Localization prob SER44		
Score diff SER44		
PEP SER44		
Score SER44		
Localization prob SER47		
Score diff SER47		
PEP SER47		
Score SER47		
Localization prob SER48		
Score diff SER48		
PEP SER48		
Score SER48		
Localization prob SER49		
Score diff SER49		

PEP SER49		
Score SER49		
Localization prob SER5		
Score diff SER5		
PEP SER5		
Score SER5		
Localization prob SER50		
Score diff SER50		
PEP SER50		
Score SER50		
Localization prob SER51		
Score diff SER51		
PEP SER51		
Score SER51		
Localization prob SER52		
Score diff SER52		
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Localization prob SER56		
Score diff SER56		
PEP SER56		
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Localization prob SER57		
Score diff SER57		
PEP SER57		
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Localization prob SER58		
Score diff SER58		
PEP SER58		
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Localization prob SER59		
Score diff SER59		
PEP SER59		
Score SER59		
Localization prob SER6		
Score diff SER6		
PEP SER6		
Score SER6		
Localization prob SER60		
Score diff SER60		
PEP SER60		
Score SER60		
Localization prob SER61		
Score diff SER61		
PEP SER61		
Score SER61		
Localization prob SER62		
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Localization prob SER63		
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PEP SER63		
Score SER63		
Localization prob SER64		
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Localization prob SER65		
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PEP SER65		
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Localization prob SER66		
Score diff SER66		
PEP SER66		
Score SER66		
Localization prob SER67		
Score diff SER67		
PEP SER67		
Score SER67		
Localization prob SER68		
Score diff SER68		
PEP SER68		
Score SER68		
Localization prob SER69		
Score diff SER69		
PEP SER69		
Score SER69		
Localization prob SER7		
Score diff SER7		
PEP SER7		
Score SER7		
Localization prob SER70		
Score diff SER70		
PEP SER70		
Score SER70		
Localization prob SER71		
Score diff SER71		
PEP SER71		
Score SER71		
Localization prob SER72		
Score diff SER72		
PEP SER72		
Score SER72		
Localization prob SER73		
Score diff SER73		
PEP SER73		
Score SER73		
Localization prob SER8		
Score diff SER8		
PEP SER8		
Score SER8		
Localization prob SER80		
Score diff SER80		
PEP SER80		
Score SER80		
Localization prob SER81		
Score diff SER81		
PEP SER81		
Score SER81		
Localization prob SER82		
Score diff SER82		
PEP SER82		
Score SER82		
Localization prob SER83		
Score diff SER83		

PEP SER83		
Score SER83		
Localization prob SER84		
Score diff SER84		
PEP SER84		
Score SER84		
Localization prob SER85		
Score diff SER85		
PEP SER85		
Score SER85		
Localization prob SER86		
Score diff SER86		
PEP SER86		
Score SER86		
Localization prob SER87		
Score diff SER87		
PEP SER87		
Score SER87		
Localization prob SER88		
Score diff SER88		
PEP SER88		
Score SER88		
Localization prob SER89		
Score diff SER89		
PEP SER89		
Score SER89		
Localization prob SER9		
Score diff SER9		
PEP SER9		
Score SER9		
Localization prob SER91		
Score diff SER91		
PEP SER91		
Score SER91		
Localization prob SER92		
Score diff SER92		
PEP SER92		
Score SER92		
Localization prob SER94		
Score diff SER94		
PEP SER94		
Score SER94		
Localization prob SER95		
Score diff SER95		
PEP SER95		
Score SER95		
Localization prob SER96		
Score diff SER96		
PEP SER96		
Score SER96		
Localization prob SER97		
Score diff SER97		
PEP SER97		
Score SER97		
Localization prob SER98		
Score diff SER98		
PEP SER98		
Score SER98		
Localization prob SER99		
Score diff SER99		
PEP SER99		
Score SER99		
Diagnostic peak		

Number of Oxidation (M)		Different numbers of Oxidation (M) on peptides that this site is involved in.
Amino acid		
Sequence window		
Modification window		
Peptide window coverage		
Oxidation (M) Probabilities		
Oxidation (M) Score diffs		
Position in peptide		
Charge		Charge state of the precursor ion.
Mass error [ppm]		Mass error of the recalibrated mass-over-charge value of the precursor ion in comparison to the predicted monoisotopic mass of the identified peptide sequence.
Identification type SER1		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER10		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER100		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER101		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER102		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER103		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER104		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER105		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER106		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER108		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER109		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER11		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER12		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER13		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER133		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER134		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER135		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER136		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER137		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER138		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER139		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER14		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER140		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER141		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER142		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER143		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER144		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER145		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER146		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER147		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER148		Indicates whether this experiment was identified by MS/MS or only by matching between runs.

Intensity SER87		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER88		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER89		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER9		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER91		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER92		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER94		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER95		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER96		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER97		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER98		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER99		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Ratio mod/base SER1		
Ratio mod/base SER10		
Ratio mod/base SER100		
Ratio mod/base SER101		
Ratio mod/base SER102		
Ratio mod/base SER103		
Ratio mod/base SER104		
Ratio mod/base SER105		
Ratio mod/base SER106		
Ratio mod/base SER108		
Ratio mod/base SER109		
Ratio mod/base SER11		
Ratio mod/base SER12		
Ratio mod/base SER13		
Ratio mod/base SER133		
Ratio mod/base SER134		
Ratio mod/base SER135		
Ratio mod/base SER136		
Ratio mod/base SER137		
Ratio mod/base SER138		
Ratio mod/base SER139		
Ratio mod/base SER14		
Ratio mod/base SER140		
Ratio mod/base SER141		
Ratio mod/base SER142		
Ratio mod/base SER143		
Ratio mod/base SER144		
Ratio mod/base SER145		

Ratio mod/base SER146		
Ratio mod/base SER147		
Ratio mod/base SER148		
Ratio mod/base SER149		
Ratio mod/base SER15		
Ratio mod/base SER150		
Ratio mod/base SER151		
Ratio mod/base SER156		
Ratio mod/base SER157		
Ratio mod/base SER160		
Ratio mod/base SER161		
Ratio mod/base SER162		
Ratio mod/base SER163		
Ratio mod/base SER164		
Ratio mod/base SER165		
Ratio mod/base SER17		
Ratio mod/base SER170		
Ratio mod/base SER171		
Ratio mod/base SER172		
Ratio mod/base SER175		
Ratio mod/base SER176		
Ratio mod/base SER177		
Ratio mod/base SER178		
Ratio mod/base SER179		
Ratio mod/base SER18		
Ratio mod/base SER180		
Ratio mod/base SER181		
Ratio mod/base SER182		
Ratio mod/base SER183		
Ratio mod/base SER184		
Ratio mod/base SER185		
Ratio mod/base SER186		
Ratio mod/base SER187		
Ratio mod/base SER19		
Ratio mod/base SER2		
Ratio mod/base SER20		
Ratio mod/base SER21		
Ratio mod/base SER23		
Ratio mod/base SER24		
Ratio mod/base SER25		
Ratio mod/base SER26		
Ratio mod/base SER27		
Ratio mod/base SER28		
Ratio mod/base SER29		
Ratio mod/base SER3		
Ratio mod/base SER30		
Ratio mod/base SER32		
Ratio mod/base SER33		
Ratio mod/base SER34		
Ratio mod/base SER35		
Ratio mod/base SER36		
Ratio mod/base SER37		
Ratio mod/base SER38		
Ratio mod/base SER39		
Ratio mod/base SER4		
Ratio mod/base SER40		
Ratio mod/base SER41		
Ratio mod/base SER42		
Ratio mod/base SER43		
Ratio mod/base SER44		
Ratio mod/base SER47		
Ratio mod/base SER48		
Ratio mod/base SER49		
Ratio mod/base SER5		

Ratio mod/base SER50		
Ratio mod/base SER51		
Ratio mod/base SER52		
Ratio mod/base SER53		
Ratio mod/base SER54		
Ratio mod/base SER55		
Ratio mod/base SER56		
Ratio mod/base SER57		
Ratio mod/base SER58		
Ratio mod/base SER59		
Ratio mod/base SER6		
Ratio mod/base SER60		
Ratio mod/base SER61		
Ratio mod/base SER62		
Ratio mod/base SER63		
Ratio mod/base SER64		
Ratio mod/base SER65		
Ratio mod/base SER66		
Ratio mod/base SER67		
Ratio mod/base SER68		
Ratio mod/base SER69		
Ratio mod/base SER7		
Ratio mod/base SER70		
Ratio mod/base SER71		
Ratio mod/base SER72		
Ratio mod/base SER73		
Ratio mod/base SER8		
Ratio mod/base SER80		
Ratio mod/base SER81		
Ratio mod/base SER82		
Ratio mod/base SER83		
Ratio mod/base SER84		
Ratio mod/base SER85		
Ratio mod/base SER86		
Ratio mod/base SER87		
Ratio mod/base SER88		
Ratio mod/base SER89		
Ratio mod/base SER9		
Ratio mod/base SER91		
Ratio mod/base SER92		
Ratio mod/base SER94		
Ratio mod/base SER95		
Ratio mod/base SER96		
Ratio mod/base SER97		
Ratio mod/base SER98		
Ratio mod/base SER99		
Intensity SER1___1		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER1___2		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER1___3		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER10___1		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER10___2		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER10___3		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.

Intensity SER97____1		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER97____2		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER97____3		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER98____1		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER98____2		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER98____3		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER99____1		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER99____2		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensity SER99____3		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Reverse		When marked with '+', this particular peptide was found to be part of a protein derived from the reversed part of the protein sequence database. These should be removed for further data analysis.
Potential contaminant		When marked with '+', this particular peptide was found to be part of a commonly occurring contaminant. These should be removed for further data analysis.
id		A unique (consecutive) identifier for each row in the site table, which is used to cross-link the information in this file with the information stored in the other files.
Protein group IDs		The identifier of the protein-group this peptide sequence is associated with, which can be used to look up the extended protein information in the file 'proteinGroups.txt'. As a single peptide can be linked to multiple proteins (e.g. in the case of razor-proteins), multiple id's can be stored here separated by a semicolon. As a protein can be identified by multiple peptides, the same id can be found in different rows.
Positions		The positions of the modifications in the protein amino acid sequence.
Position		The position of the modification in the protein amino acid sequence.
Peptide IDs		Identifier(s) of the associated peptide sequence(s) summary, which can be found in the file 'peptides.txt'.
Mod. peptide IDs		Identifier(s) of the associated peptide sequence(s) summary, which can be found in the file 'modificationSpecificPeptides.txt'.
Evidence IDs		Identifier(s) for analyzed peptide evidence associated with the protein group referenced against the evidence table.
MS/MS IDs		The identifiers of the MS/MS scans identifying this peptide, referenced against the msms table.
Best localization evidence ID		
Best localization MS/MS ID		
Best localization raw file		
Best localization scan number		
Best score evidence ID		
Best score MS/MS ID		
Best score raw file		
Best score scan number		
Best PEP evidence ID		
Best PEP MS/MS ID		
Best PEP raw file		
Best PEP scan number		

Protein groups

The Protein Groups table contains information on the identified proteins in the processed raw-files. Each single row contains the group of proteins that could be reconstructed from a set of peptides.

Name	Separator	Description
Protein IDs		Identifiers of proteins contained in the protein group. They are sorted by number of identified peptides in descending order.
Majority protein IDs		These are the IDs of those proteins that have at least half of the peptides that the leading protein has.
Peptide counts (all)		Number of peptides associated with each protein in protein group, occurring in the order as the protein IDs occur in the 'Protein IDs' column. Here distinct peptide sequences are counted. Modified forms or different charges are counted as one peptide.
Peptide counts (razor+unique)		Number of peptides associated with each protein in protein group, occurring in the order as the protein IDs occur in the 'Protein IDs' column. Here distinct peptide sequences are counted. Modified forms or different charges are counted as one peptide.
Peptide counts (unique)		Number of peptides associated with each protein in protein group, occurring in the order as the protein IDs occur in the 'Protein IDs' column. Here distinct peptide sequences are counted. Modified forms or different charges are counted as one peptide.
Fasta headers		Fasta headers(s) of protein(s) contained within the group.
Number of proteins		Number of proteins contained within the group. This corresponds to the number of entries in the column 'Protein IDs'.
Peptides		The total number of peptide sequences associated with the protein group (i.e. for all the proteins in the group).
Razor + unique peptides		The total number of razor + unique peptides associated with the protein group (i.e. these peptides are shared with another protein group).
Unique peptides		The total number of unique peptides associated with the protein group (i.e. these peptides are not shared with another protein group).
Peptides SER1		Number of peptides (distinct peptide sequences) in experiment SER1
Peptides SER10		Number of peptides (distinct peptide sequences) in experiment SER10
Peptides SER100		Number of peptides (distinct peptide sequences) in experiment SER100
Peptides SER101		Number of peptides (distinct peptide sequences) in experiment SER101
Peptides SER102		Number of peptides (distinct peptide sequences) in experiment SER102
Peptides SER103		Number of peptides (distinct peptide sequences) in experiment SER103
Peptides SER104		Number of peptides (distinct peptide sequences) in experiment SER104
Peptides SER105		Number of peptides (distinct peptide sequences) in experiment SER105
Peptides SER106		Number of peptides (distinct peptide sequences) in experiment SER106
Peptides SER108		Number of peptides (distinct peptide sequences) in experiment SER108
Peptides SER109		Number of peptides (distinct peptide sequences) in experiment SER109
Peptides SER11		Number of peptides (distinct peptide sequences) in experiment SER11
Peptides SER12		Number of peptides (distinct peptide sequences) in experiment SER12
Peptides SER13		Number of peptides (distinct peptide sequences) in experiment SER13
Peptides SER133		Number of peptides (distinct peptide sequences) in experiment SER133
Peptides SER134		Number of peptides (distinct peptide sequences) in experiment SER134
Peptides SER135		Number of peptides (distinct peptide sequences) in experiment SER135
Peptides SER136		Number of peptides (distinct peptide sequences) in experiment SER136

Unique peptides SER83		Number of unique peptides (distinct peptide sequences) in experiment SER83
Unique peptides SER84		Number of unique peptides (distinct peptide sequences) in experiment SER84
Unique peptides SER85		Number of unique peptides (distinct peptide sequences) in experiment SER85
Unique peptides SER86		Number of unique peptides (distinct peptide sequences) in experiment SER86
Unique peptides SER87		Number of unique peptides (distinct peptide sequences) in experiment SER87
Unique peptides SER88		Number of unique peptides (distinct peptide sequences) in experiment SER88
Unique peptides SER89		Number of unique peptides (distinct peptide sequences) in experiment SER89
Unique peptides SER9		Number of unique peptides (distinct peptide sequences) in experiment SER9
Unique peptides SER91		Number of unique peptides (distinct peptide sequences) in experiment SER91
Unique peptides SER92		Number of unique peptides (distinct peptide sequences) in experiment SER92
Unique peptides SER94		Number of unique peptides (distinct peptide sequences) in experiment SER94
Unique peptides SER95		Number of unique peptides (distinct peptide sequences) in experiment SER95
Unique peptides SER96		Number of unique peptides (distinct peptide sequences) in experiment SER96
Unique peptides SER97		Number of unique peptides (distinct peptide sequences) in experiment SER97
Unique peptides SER98		Number of unique peptides (distinct peptide sequences) in experiment SER98
Unique peptides SER99		Number of unique peptides (distinct peptide sequences) in experiment SER99
Sequence coverage [%]		Percentage of the sequence that is covered by the identified peptides of the best protein sequence contained in the group.
Unique + razor sequence coverage [%]		Percentage of the sequence that is covered by the identified unique and razor peptides of the best protein sequence contained in the group.
Unique sequence coverage [%]		Percentage of the sequence that is covered by the identified unique peptides of the best protein sequence contained in the group.
Mol. weight [kDa]		Molecular weight of the leading protein sequence contained in the protein group.
Sequence length		The length of the leading protein sequence contained in the group.
Sequence lengths		The length of all sequences of the proteins contained in the group.
Fraction average		
Fraction 1		
Fraction 2		
Fraction 3		
Fraction 10		
Q-value		This is the ratio of reverse to forward protein groups.
Score		Protein score which is derived from peptide posterior error probabilities.
Identification type SER1		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER10		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER100		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER101		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER102		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER103		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER104		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER105		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER106		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER108		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SER109		Indicates whether this experiment was identified by MS/MS or only by matching between runs.

Intensity SER99		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
iBAQ		
iBAQ SER1		
iBAQ SER10		
iBAQ SER100		
iBAQ SER101		
iBAQ SER102		
iBAQ SER103		
iBAQ SER104		
iBAQ SER105		
iBAQ SER106		
iBAQ SER108		
iBAQ SER109		
iBAQ SER11		
iBAQ SER12		
iBAQ SER13		
iBAQ SER133		
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LFQ intensity SER60		
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LFQ intensity SER72		
LFQ intensity SER73		
LFQ intensity SER91		
LFQ intensity SER92		
LFQ intensity SER94		
MS/MS count SER105		
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MS/MS count SER72		
MS/MS count SER73		
MS/MS count SER91		
MS/MS count SER92		
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LFQ intensity SER1		
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LFQ intensity SER100		
LFQ intensity SER101		
LFQ intensity SER102		
LFQ intensity SER103		
LFQ intensity SER104		
LFQ intensity SER133		
LFQ intensity SER134		
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LFQ intensity SER99		
MS/MS count SER1		
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MS/MS count SER98		
MS/MS count SER99		
MS/MS count		
Only identified by site		When marked with '+', this particular protein group was identified only by a modification site.
Reverse		When marked with '+', this particular protein group contains no protein, made up of at least 50% of the peptides of the leading protein, with a peptide derived from the reversed part of the decoy database. These should be removed for further data analysis. The 50% rule is in place to prevent spurious protein hits to erroneously flag the protein group as reverse.
Potential contaminant		When marked with '+', this particular protein group was found to be a commonly occurring contaminant. These should be removed for further data analysis.
id		A unique (consecutive) identifier for each row in the proteinGroups table, which is used to cross-link the information in this file with the information stored in the other files.
Peptide IDs		Identifier(s) of the associated peptide sequence(s) summary, which can be found in the file 'peptides.txt'.
Peptide is razor		Indicates for each peptide ID if it is a razor or group unique peptide (true) or a non unique non razor peptide (false).
Mod. peptide IDs		
Evidence IDs		
MS/MS IDs		
Best MS/MS		The identifier of the best (in terms of quality) MS/MS scans identifying the peptides of this protein, referenced against the msms table.
Deamidation (NQ) site IDs		Identifier(s) for site(s) associated with the protein group, which show(s) evidence of the modification, referenced against the appropriate modification site file.
Oxidation (M) site IDs		Identifier(s) for site(s) associated with the protein group, which show(s) evidence of the modification, referenced against the appropriate modification site file.
Deamidation (NQ) site positions		Positions of the sites in the leading protein of this group.
Oxidation (M) site positions		Positions of the sites in the leading protein of this group.

All peptides

Name	Separator	Description
Raw file		Name of the raw file the spectral data was extracted from.
Type		The type of detection for the peptide. MULTI – A labeling multiplet was detected. ISO – An isotope pattern was detected.
Charge		The charge state of the peptide.
m/z		The mass divided by the charge of the charged peptide.
Mass		The mass of the neutral peptide ((m/z-proton) * charge).
Uncalibrated m/z		m/z before re-calibrations have been applied.
Resolution		The resolution of the peak detected for the peptide measured in Full Width at Half Maximum (FWHM).
Number of data points		The number of data points (peak centroids) collected for this peptide feature.
Number of scans		The number of MS scans that the 3d peaks of this peptide feature are overlapping with.
Number of isotopic peaks		The number of isotopic peaks contained in this peptide feature.
PIF		Short for Parent Ion Fraction; indicates the fraction the target peak makes up of the total intensity in the inclusion window.
Mass fractional part		The values after the radix point (ie value - floor(value)).
Mass deficit		Empirically derived deviation measure to the next nearest integer scaled to center around 0. Can be used to visually detect contaminants in a plot setting Mass against this value. $m*a+b - \text{round}(m*a+b)$ m: the peptide mass a: 0.99954 b: -0.04
Mass precision [ppm]		The precision of the mass detection of the peptide in parts-per-million.
Max intensity m/z 0		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Retention time		The retention time of the peak detected for the peptide measured in minutes.
Retention length		The total retention time width of the peak (last time point – first time point) in seconds.
Retention length (FWHM)		The full width at half maximum value retention time width of the peak in seconds.
Min scan number		The first scan number at which the peak was encountered.
Max scan number		The last scan number at which the peak was encountered.
Identified		When marked with '+' this particular MS/MS scan was identified as a peptide; when marked with '-' no identification was made.
MS/MS IDs		Unique identifier linking this identification to the MS/MS scans.
Sequence		The identified AA sequence of the peptide.
Length		The length of the sequence stored in the column "Sequence".
Modifications		Post-translational modifications contained within the sequence. When no modifications exist, this is set to 'unmodified'. Note: This column only set when this MS/MS spectrum has been identified.
Modified sequence		Sequence representation of the peptide including location(s) of modified AAs. Note: This column only set when this MS/MS spectrum has been identified.
Proteins		Identifiers of proteins this peptide is associated with. Note: This column only set when this MS/MS spectrum has been identified.
Score		The score of the identification (higher is better). Note: This column only set when this MS/MS spectrum has been identified.
Intensity		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensities		Elution profile.
Isotope pattern		Isotope pattern.

MS/MS Count		The number of MS/MS spectra recorded for the peptide.
MSMS Scan Numbers		The scan numbers where the MS/MS spectra were recorded.
MSMS Isotope Indices		Indices of the isotopic peaks that the MS/MS spectra reside on. A value of 0 corresponds to the monoisotopic peak.

MS scans

The msScans table contains information about the full scans, which can be used to verify data quality and generated useful statistics about the interaction between the samples and LC.

Name	Separator	Description
Raw file		The name of the RAW-file the mass spectral data originates from.
Scan number		The scan number (defined in the raw-file) at which the full scan was made.
Scan index		The consecutive index of this full scan.
Retention time		The retention time at which the full scan was made.
Cycle time		The total time (full scan including the tandem MS scans) this full scan has taken up.
Ion injection time		The total injection time that was required to capture the specified amount of ions. This value is limited by a maximum, which can be used to determine whether the time has maxed out (indicative of a bad acquisition).
Base peak intensity		The intensity of the most intense ion in the spectrum.
Total ion current		The total intensity acquired in the full scan.
MS/MS count		The number of tandem MS scans that were made based on this full scan (e.g. a top 10 method selects the top 10 most intense ions in the scan and fragments those).
Mass calibration		The applied mass correction in Th to the full scan.
Fraction		The fraction measured with this full scan.
Experiment		
Peak length		The average time between the start and the end of the peaks detected in the full scan.
Isotope pattern length		The average time between the start and the end of the isotope patterns detected in the full scan.
Multiplet length		The average time between the start and the end of the isotope patterns of the labeling multiplets detected in the full scan.
Peaks / s		The average number of peaks detected per second of chromatography.
Single peaks / s		The average number of single peaks detected per second of chromatography.
Isotope patterns / s		The average number of isotope patterns detected per second of chromatography.
Single isotope patterns / s		The average number of single isotope patterns detected per second of chromatography.
Multiplets / s		The average number of labeling multiplets detected per second of chromatography.
Identified multiplets / s		The percentage of labeling multiplets actually identified.
Multiplet identification rate [%]		The percentage of the detected labeling multiplets that were identified.
MS/MS / s		The average number of MS/MS events per second of chromatography.
Identified MS/MS / s		The average number of identified MS/MS events per second of chromatography.
MS/MS identification rate [%]		The percentage of tandem MS scans that were identified.
Intens Comp Factor		Taken from the Thermo RAW file.
CTCD Comp		Taken from the Thermo RAW file.
RawOvFtT		For Thermo Fisher only. TIC estimation done with the orbitrap cell.
AGC Fill		Taken from the Thermo RAW file.

MZ range

Name	Separator	Description
Raw file		The name of the RAW-file the mass spectral data was derived from.
m/z		The mass-over-charge value.
Peaks / Da		The average number of peaks detected per Dalton.
Single peaks / Da		The average number of single peaks detected per Dalton.
Isotope patterns / Da		The average number of isotope patterns detected per Dalton.
Single isotope patterns / Da		The average number of single isotope patterns detected per Dalton.
SILAC pairs / Da		The average number of SILAC pairs detected per Dalton.
Identified SILAC pairs / Da		The percentage of SILAC pairs actually identified.
SILAC identification rate [%]		The percentage of the detected SILAC pairs that were identified.
MS/MS / Da		The average number of MS/MS events per Dalton.
Identified MS/MS / Da		The average number of identified MS/MS events per Dalton.
Identification rate [%]		The percentage of tandem MS scans that were identified.

MS/MS scans

Name	Separator	Description
Raw file		Name of the RAW file the spectral MS/MS data was extracted from.
Scan number		RAW file derived scan number for the MS/MS spectrum.
Retention time		Time point along the elution profile at which the MS/MS data was recorded.
Ion injection time		The ion inject time for the MS/MS scan. This can be used to determine if this time equals to the maximum ion inject time, general indicative of a lower quality spectrum.
Total ion current		The total ion current of the MS/MS scan. For Thermo data this value is calculated by summing all the intensity values found in the mass spectral data, which is different from the Xcalibur reported TIC (Xcalibur TIC is about 25% of the value reported here).
Collision energy		The collision energy used for the fragmentation that resulted in this MS/MS scan.
Summations		For time of flight instruments only.
Base peak intensity		The intensity of the most intense ion in the spectrum.
Elapsed time		The time the MS/MS scan took to complete.
Identified		When marked with '+' this particular MS/MS scan was identified as a peptide; when marked with '-' no identification was made.
MS/MS IDs		Unique identifier linking this identification to the MS/MS scans.
Sequence		The identified AA sequence of the peptide.
Length		The length of the sequence stored in the column "Sequence".
Filtered peaks		Number of peaks after the 'top X per 100 Da' filtering.
m/z		Recalibrated m/z of the precursor ion.
Mass		Charge corrected mass of the precursor ion.
Charge		Charge state of the precursor ion.
Type		The type of precursor ion as identified by MaxQuant. ISO – isotopic cluster. PEAK – single peak. MULTI – labeling cluster.
Fragmentation		The type of fragmentation used to create the MS/MS spectrum. CID – Collision Induced Dissociation. HCD – High energy Collision induced Dissociation. ETD – Electron Transfer Dissociation.
Mass analyzer		The mass analyzer used to record the MS/MS spectrum. ITMS – Ion trap. FTMS – Fourier transform ICR or orbitrap cell. TOF – Time of flight.
Parent intensity fraction		The percentage the parent ion intensity makes up of the total intensity in the selection window.
Fraction of total spectrum		The percentage the parent ion intensity makes up of the total intensity of the whole MS spectrum.
Base peak fraction		The percentage the parent ion intensity in comparison to the highest peak in the MS spectrum.
Precursor full scan number		The full scan number where the precursor ion was selected for fragmentation.
Precursor intensity		The intensity of the precursor ion at the scan number it was selected.
Precursor apex fraction		The fraction the intensity of the precursor ion makes up of the peak (apex) intensity.
Precursor apex offset		How many full scans the precursor ion is offset from the peak (apex) position.
Precursor apex offset time		How much time the precursor ion is offset from the peak (apex) position.
Scan event number		This number indicates which MS/MS scan this one is in the consecutive order of the MS/MS scans that are acquired after an MS scan.
Modifications		Post-translational modifications contained within the sequence. When no modifications exist, this is set to 'unmodified'. Note: This column only set when this MS/MS spectrum has been identified.
Modified sequence		Sequence representation of the peptide including location(s) of modified AAs. Note: This column only set when this MS/MS spectrum has been identified.

Proteins		Identifiers of proteins this peptide is associated with. Note: This column only set when this MS/MS spectrum has been identified.
Score		The score of the identification (higher is better). Note: This column only set when this MS/MS spectrum has been identified.
Fraction		The identifier of the fraction the sample was taken from.
Experiment		
Reporter PIF		
Reporter fraction		
Intens Comp Factor		Taken from the Thermo RAW file.
CTCD Comp		Taken from the Thermo RAW file.
RawOvFtT		For Thermo Fisher only. TIC estimation done with the orbitrap cell.
AGC Fill		Taken from the Thermo RAW file.
Scan index		Consecutive index of the MS/MS spectrum.
MS scan index		Consecutive index of the MS spectrum prior to this MS/MS spectrum.
MS scan number		Scan number of the MS spectrum prior to this MS/MS spectrum.

MS/MS

Name	Separator	Description
Raw file		The name of the RAW file the mass spectral data was read from.
Scan number		The RAW-file derived scan number of the MS/MS spectrum.
Scan index		The consecutive index of the MS/MS spectrum.
Sequence		The identified AA sequence of the peptide.
Length		The length of the sequence stored in the column "Sequence".
Missed cleavages		Number of missed enzymatic cleavages.
Modifications		Post-translational modifications contained within the identified peptide sequence.
Modified sequence		Sequence representation including the post-translational modifications (abbreviation of the modification in brackets before the modified AA). The sequence is always surrounded by underscore characters ('_').
Deamidation (NQ) Probabilities		Sequence representation of the peptide including PTM positioning probabilities ([0..1], where 1 is best match) for 'Deamidation (NQ)'. Example: <code>Q[0.1]K</code>
Oxidation (M) Probabilities		Sequence representation of the peptide including PTM positioning probabilities ([0..1], where 1 is best match) for 'Oxidation (M)'. Example: <code>M[0.1]K</code>
Deamidation (NQ) Score diffs		
Oxidation (M) Score diffs		
Acetyl (Protein N-term)		
Deamidation (NQ)		
Oxidation (M)		
Proteins		The identifiers of the proteins the identified peptide is associated with.
Charge		The charge state of the precursor ion.
Fragmentation		The type of fragmentation used to create the MS/MS spectrum. CID – Collision Induced Dissociation. HCD – High energy Collision induced Dissociation. ETD – Electron Transfer Dissociation.
Mass analyzer		The mass analyzer used to record the MS/MS spectrum. ITMS – Ion trap. FTMS – Fourier transform ICR or orbitrap cell. TOF – Time of flight.
Type		The type of precursor ion as identified by MaxQuant. ISO – isotopic cluster. PEAK – single peak. MULTI – labeling cluster.
Scan event number		
Isotope index		
m/z		The mass-over-charge of the precursor ion.
Mass		The charge corrected mass of the precursor ion.
Mass error [ppm]		Mass error of the recalibrated mass-over-charge value of the precursor ion in comparison to the predicted monoisotopic mass of the identified peptide sequence expressed in parts per million.
Mass error [Da]		Mass error of the recalibrated mass-over-charge value of the precursor ion in comparison to the predicted monoisotopic mass of the identified peptide sequence expressed in atomic mass units.
Simple mass error [ppm]		
Retention time		The uncalibrated retention time in minutes where the MS/MS spectrum has been acquired.
PEP		Posterior Error Probability of the identification. This value essentially operates as a p-value, where smaller is more significant.
Score		Andromeda score for the best associated MS/MS spectrum.
Delta score		Score difference to the second best identified peptide with a different amino acid sequence.
Score diff		Score difference to the second best positioning of modifications identified peptide with the same amino acid sequence.
Localization prob		
Combinatorics		Number of possible distributions of the modifications over the peptide sequence.
PIF		Short for Parent Ion Fraction; indicates the fraction the target peak makes up of the total intensity in the inclusion window.

Fraction of total spectrum		The percentage the parent ion intensity makes up of the total intensity of the whole spectrum.
Base peak fraction		The percentage the parent ion intensity in comparison to the highest peak in the MS spectrum.
Precursor full scan number		The full scan number where the precursor ion was selected for fragmentation.
Precursor Intensity		The intensity of the precursor ion at the scan number it was selected.
Precursor apex fraction		The fraction the intensity of the precursor ion makes up of the peak (apex) intensity.
Precursor apex offset		How many full scans the precursor ion is offset from the peak (apex) position.
Precursor apex offset time		How much time the precursor ion is offset from the peak (apex) position.
Matches		The species of the peaks in the fragmentation spectrum after TopN filtering.
Intensities		The intensities of the peaks in the fragmentation spectrum after TopN filtering.
Mass deviations [Da]		The mass deviation of each peak in the fragmentation spectrum in absolute mass units.
Mass deviations [ppm]		The mass deviation of each peak in the fragmentation spectrum in parts per million.
Masses		The masses-over-charge of the peaks in the fragmentation spectrum.
Number of matches		The number of peaks matching to the predicted fragmentation spectrum.
Intensity coverage		The fraction of intensity in the MS/MS spectrum that is annotated.
Peak coverage		The fraction of peaks in the MS/MS spectrum that are annotated.
Neutral loss level		How many neutral losses were applied to each fragment in the Andromeda scoring.
ETD identification type		For ETD spectra several different combinations of ion series are scored. Here the highest scoring combination is indicated
Reverse		When marked with '+', this particular peptide was found to be part of a protein derived from the reversed part of the decoy database. These should be removed for further data analysis.
All scores		
All sequences		
All modified sequences		
Reporter PIF		
Reporter fraction		
id		A unique (consecutive) identifier for each row in the msms table, which is used to cross-link the information in this file with the information stored in the other files.
Protein group IDs		The identifier of the protein-group this redundant peptide sequence is associated with, which can be used to look up the extended protein information in the file 'proteinGroups.txt'. As a single peptide can be linked to multiple proteins (e.g. in the case of razor-proteins), multiple id's can be stored here separated by a semicolon. As a protein can be identified by multiple peptides, the same id can be found in different rows.
Peptide ID		The identifier of the non-redundant peptide sequence.
Mod. peptide ID		Identifier of the associated modification summary stored in the file 'modificationSpecificPeptides.txt'.
Evidence ID		Identifier of the associated evidence stored in the file 'evidence.txt'.
Deamidation (NQ) site IDs		Identifier of the associated entry stored in the file 'Deamidation (NQ)Sites.txt'.
Oxidation (M) site IDs		Identifier of the associated entry stored in the file 'Oxidation (M)Sites.txt'.