

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.
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 ('_').
NEM_free_CAA Probabilities		Sequence representation of the peptide including PTM positioning probabilities ([0..1], where 1 is best match) for 'NEM_free_CAA'.
Oxidation (M) Probabilities		Sequence representation of the peptide including PTM positioning probabilities ([0..1], where 1 is best match) for 'Oxidation (M)'.
NEM_free_CAA 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)'.
NEM_free_CAA		The number of occurrences of the modification 'NEM_free_CAA'.
Oxidation (M)		The number of occurrences of the modification 'Oxidation (M)'.
Missed cleavages (AspN)		Number of missed enzymatic cleavages.
Missed cleavages (AspN;GluC_phos)		Number of missed enzymatic cleavages.
Missed cleavages (Chymotrypsin+)		Number of missed enzymatic cleavages.
Missed cleavages (Trypsin/P)		Number of missed enzymatic cleavages.
Missed cleavages (Trypsin/P;AspN)		Number of missed enzymatic cleavages.
Missed cleavages (GluC_phos)		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.
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.

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.
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'.
NEM_free_CAA site IDs		Identifier(s) of the modification summary stored in the file 'NEM_free_CAASites.txt'.
Oxidation (M) site IDs		Identifier(s) of the modification summary stored in the file 'Oxidation (M)Sites.txt'.
Taxonomy IDs		Taxonomy identifiers.

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 (AspN)		Number of missed enzymatic cleavages.
Missed cleavages (AspN;GluC_phos)		Number of missed enzymatic cleavages.
Missed cleavages (Chymotrypsin+)		Number of missed enzymatic cleavages.
Missed cleavages (Trypsin/P)		Number of missed enzymatic cleavages.
Missed cleavages (Trypsin/P;AspN)		Number of missed enzymatic cleavages.
Missed cleavages (GluC_phos)		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 NEM_01		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_02		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_03		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_04		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_05		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_06		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_07		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_08		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_09		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_10		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_11		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_12		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_13		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_14		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_15		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_16		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SS_01		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SS_02		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SS_03		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SS_04		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SS_05		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SS_06		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SS_07		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SS_08		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SS_09		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SS_10		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SS_11		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SS_12		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SS_13		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SS_14		Indicates whether this experiment was identified by MS/MS or only by matching between runs.

Identification type SS_15		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SS_16		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Experiment NEM_01		Number of evidence entries for this 'Experiment'.
Experiment NEM_02		Number of evidence entries for this 'Experiment'.
Experiment NEM_03		Number of evidence entries for this 'Experiment'.
Experiment NEM_04		Number of evidence entries for this 'Experiment'.
Experiment NEM_05		Number of evidence entries for this 'Experiment'.
Experiment NEM_06		Number of evidence entries for this 'Experiment'.
Experiment NEM_07		Number of evidence entries for this 'Experiment'.
Experiment NEM_08		Number of evidence entries for this 'Experiment'.
Experiment NEM_09		Number of evidence entries for this 'Experiment'.
Experiment NEM_10		Number of evidence entries for this 'Experiment'.
Experiment NEM_11		Number of evidence entries for this 'Experiment'.
Experiment NEM_12		Number of evidence entries for this 'Experiment'.
Experiment NEM_13		Number of evidence entries for this 'Experiment'.
Experiment NEM_14		Number of evidence entries for this 'Experiment'.
Experiment NEM_15		Number of evidence entries for this 'Experiment'.
Experiment NEM_16		Number of evidence entries for this 'Experiment'.
Experiment SS_01		Number of evidence entries for this 'Experiment'.
Experiment SS_02		Number of evidence entries for this 'Experiment'.
Experiment SS_03		Number of evidence entries for this 'Experiment'.
Experiment SS_04		Number of evidence entries for this 'Experiment'.
Experiment SS_05		Number of evidence entries for this 'Experiment'.
Experiment SS_06		Number of evidence entries for this 'Experiment'.
Experiment SS_07		Number of evidence entries for this 'Experiment'.
Experiment SS_08		Number of evidence entries for this 'Experiment'.
Experiment SS_09		Number of evidence entries for this 'Experiment'.
Experiment SS_10		Number of evidence entries for this 'Experiment'.
Experiment SS_11		Number of evidence entries for this 'Experiment'.
Experiment SS_12		Number of evidence entries for this 'Experiment'.
Experiment SS_13		Number of evidence entries for this 'Experiment'.
Experiment SS_14		Number of evidence entries for this 'Experiment'.
Experiment SS_15		Number of evidence entries for this 'Experiment'.
Experiment SS_16		Number of evidence entries for this 'Experiment'.
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 NEM_01		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 NEM_02		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 NEM_03		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 NEM_04		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 NEM_05		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 NEM_06		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 NEM_07		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 NEM_08		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 SS_14		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 SS_15		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 SS_16		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.
NEM_free_CAA 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.
Taxonomy IDs		Taxonomy identifiers.
MS/MS Count		
LFQ intensity NEM_01		
LFQ intensity NEM_02		
LFQ intensity NEM_03		
LFQ intensity NEM_04		
LFQ intensity NEM_05		
LFQ intensity NEM_06		
LFQ intensity NEM_07		
LFQ intensity NEM_08		
LFQ intensity NEM_09		
LFQ intensity NEM_10		
LFQ intensity NEM_11		
LFQ intensity NEM_12		
LFQ intensity NEM_13		
LFQ intensity NEM_14		
LFQ intensity NEM_15		
LFQ intensity NEM_16		
LFQ intensity SS_01		
LFQ intensity SS_02		
LFQ intensity SS_03		
LFQ intensity SS_04		
LFQ intensity SS_05		
LFQ intensity SS_06		
LFQ intensity SS_07		
LFQ intensity SS_08		
LFQ intensity SS_09		
LFQ intensity SS_10		
LFQ intensity SS_11		
LFQ intensity SS_12		
LFQ intensity SS_13		
LFQ intensity SS_14		
LFQ intensity SS_15		
LFQ intensity SS_16		

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.
NEM_free_CAA		Number of NEM_free_CAA on this peptide.
Oxidation (M)		Number of Oxidation (M) on this peptide.
Missed cleavages (AspN)		Number of missed enzymatic cleavages.
Missed cleavages (AspN;GluC_phos)		Number of missed enzymatic cleavages.
Missed cleavages (Chymotrypsin+)		Number of missed enzymatic cleavages.
Missed cleavages (Trypsin/P)		Number of missed enzymatic cleavages.
Missed cleavages (Trypsin/P;AspN)		Number of missed enzymatic cleavages.
Missed cleavages (GluC_phos)		Number of missed enzymatic cleavages.
Identification type NEM_01		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_02		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_03		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_04		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_05		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_06		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_07		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_08		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_09		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_10		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_11		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_12		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_13		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_14		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_15		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_16		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SS_01		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SS_02		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SS_03		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SS_04		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SS_05		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SS_06		Indicates whether this experiment was identified by MS/MS or only by matching between runs.

Identification type SS_07		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SS_08		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SS_09		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SS_10		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SS_11		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SS_12		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SS_13		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SS_14		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SS_15		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SS_16		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Experiment NEM_01		Number of evidence entries for this 'Experiment'.
Experiment NEM_02		Number of evidence entries for this 'Experiment'.
Experiment NEM_03		Number of evidence entries for this 'Experiment'.
Experiment NEM_04		Number of evidence entries for this 'Experiment'.
Experiment NEM_05		Number of evidence entries for this 'Experiment'.
Experiment NEM_06		Number of evidence entries for this 'Experiment'.
Experiment NEM_07		Number of evidence entries for this 'Experiment'.
Experiment NEM_08		Number of evidence entries for this 'Experiment'.
Experiment NEM_09		Number of evidence entries for this 'Experiment'.
Experiment NEM_10		Number of evidence entries for this 'Experiment'.
Experiment NEM_11		Number of evidence entries for this 'Experiment'.
Experiment NEM_12		Number of evidence entries for this 'Experiment'.
Experiment NEM_13		Number of evidence entries for this 'Experiment'.
Experiment NEM_14		Number of evidence entries for this 'Experiment'.
Experiment NEM_15		Number of evidence entries for this 'Experiment'.
Experiment NEM_16		Number of evidence entries for this 'Experiment'.
Experiment SS_01		Number of evidence entries for this 'Experiment'.
Experiment SS_02		Number of evidence entries for this 'Experiment'.
Experiment SS_03		Number of evidence entries for this 'Experiment'.
Experiment SS_04		Number of evidence entries for this 'Experiment'.
Experiment SS_05		Number of evidence entries for this 'Experiment'.
Experiment SS_06		Number of evidence entries for this 'Experiment'.
Experiment SS_07		Number of evidence entries for this 'Experiment'.
Experiment SS_08		Number of evidence entries for this 'Experiment'.
Experiment SS_09		Number of evidence entries for this 'Experiment'.
Experiment SS_10		Number of evidence entries for this 'Experiment'.
Experiment SS_11		Number of evidence entries for this 'Experiment'.
Experiment SS_12		Number of evidence entries for this 'Experiment'.
Experiment SS_13		Number of evidence entries for this 'Experiment'.
Experiment SS_14		Number of evidence entries for this 'Experiment'.
Experiment SS_15		Number of evidence entries for this 'Experiment'.
Experiment SS_16		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.

Intensity SS_03		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 SS_04		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 SS_05		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 SS_06		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 SS_07		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 SS_08		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 SS_09		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 SS_10		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 SS_11		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 SS_12		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 SS_13		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 SS_14		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 SS_15		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 SS_16		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.
NEM_free_CAA 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		
Taxonomy IDs		Taxonomy identifiers.

NEM_free_CAASites

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 NEM_01		
Score diff NEM_01		
PEP NEM_01		
Score NEM_01		
Localization prob NEM_02		
Score diff NEM_02		
PEP NEM_02		
Score NEM_02		
Localization prob NEM_03		
Score diff NEM_03		
PEP NEM_03		
Score NEM_03		
Localization prob NEM_04		
Score diff NEM_04		
PEP NEM_04		
Score NEM_04		
Localization prob NEM_05		
Score diff NEM_05		
PEP NEM_05		
Score NEM_05		
Localization prob NEM_06		
Score diff NEM_06		
PEP NEM_06		
Score NEM_06		
Localization prob NEM_07		
Score diff NEM_07		
PEP NEM_07		
Score NEM_07		
Localization prob NEM_08		
Score diff NEM_08		
PEP NEM_08		
Score NEM_08		
Localization prob NEM_09		
Score diff NEM_09		
PEP NEM_09		
Score NEM_09		
Localization prob NEM_10		
Score diff NEM_10		
PEP NEM_10		
Score NEM_10		
Localization prob NEM_11		
Score diff NEM_11		

PEP NEM_11		
Score NEM_11		
Localization prob NEM_12		
Score diff NEM_12		
PEP NEM_12		
Score NEM_12		
Localization prob NEM_13		
Score diff NEM_13		
PEP NEM_13		
Score NEM_13		
Localization prob NEM_14		
Score diff NEM_14		
PEP NEM_14		
Score NEM_14		
Localization prob NEM_15		
Score diff NEM_15		
PEP NEM_15		
Score NEM_15		
Localization prob NEM_16		
Score diff NEM_16		
PEP NEM_16		
Score NEM_16		
Localization prob SS_01		
Score diff SS_01		
PEP SS_01		
Score SS_01		
Localization prob SS_02		
Score diff SS_02		
PEP SS_02		
Score SS_02		
Localization prob SS_03		
Score diff SS_03		
PEP SS_03		
Score SS_03		
Localization prob SS_04		
Score diff SS_04		
PEP SS_04		
Score SS_04		
Localization prob SS_05		
Score diff SS_05		
PEP SS_05		
Score SS_05		
Localization prob SS_06		
Score diff SS_06		
PEP SS_06		
Score SS_06		
Localization prob SS_07		
Score diff SS_07		
PEP SS_07		
Score SS_07		
Localization prob SS_08		
Score diff SS_08		
PEP SS_08		
Score SS_08		
Localization prob SS_09		
Score diff SS_09		
PEP SS_09		
Score SS_09		
Localization prob SS_10		
Score diff SS_10		
PEP SS_10		
Score SS_10		
Localization prob SS_11		
Score diff SS_11		

PEP SS_11		
Score SS_11		
Localization prob SS_12		
Score diff SS_12		
PEP SS_12		
Score SS_12		
Localization prob SS_13		
Score diff SS_13		
PEP SS_13		
Score SS_13		
Localization prob SS_14		
Score diff SS_14		
PEP SS_14		
Score SS_14		
Localization prob SS_15		
Score diff SS_15		
PEP SS_15		
Score SS_15		
Localization prob SS_16		
Score diff SS_16		
PEP SS_16		
Score SS_16		
Diagnostic peak		
Number of NEM_free_CAA		Different numbers of NEM_free_CAA on peptides that this site is involved in.
Amino acid		
Sequence window		
Modification window		
Peptide window coverage		
NEM_free_CAA Probabilities		
NEM_free_CAA 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 NEM_01		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_02		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_03		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_04		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_05		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_06		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_07		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_08		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_09		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_10		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_11		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_12		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_13		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_14		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_15		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_16		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SS_01		Indicates whether this experiment was identified by MS/MS or only by matching between runs.

Intensity SS_14		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 SS_15		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 SS_16		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 NEM_01		
Ratio mod/base NEM_02		
Ratio mod/base NEM_03		
Ratio mod/base NEM_04		
Ratio mod/base NEM_05		
Ratio mod/base NEM_06		
Ratio mod/base NEM_07		
Ratio mod/base NEM_08		
Ratio mod/base NEM_09		
Ratio mod/base NEM_10		
Ratio mod/base NEM_11		
Ratio mod/base NEM_12		
Ratio mod/base NEM_13		
Ratio mod/base NEM_14		
Ratio mod/base NEM_15		
Ratio mod/base NEM_16		
Ratio mod/base SS_01		
Ratio mod/base SS_02		
Ratio mod/base SS_03		
Ratio mod/base SS_04		
Ratio mod/base SS_05		
Ratio mod/base SS_06		
Ratio mod/base SS_07		
Ratio mod/base SS_08		
Ratio mod/base SS_09		
Ratio mod/base SS_10		
Ratio mod/base SS_11		
Ratio mod/base SS_12		
Ratio mod/base SS_13		
Ratio mod/base SS_14		
Ratio mod/base SS_15		
Ratio mod/base SS_16		
Intensity NEM_01___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 NEM_01___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 NEM_01___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 NEM_02___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 NEM_02___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 NEM_02___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 NEM_03___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 SS_15___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 SS_15___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 SS_16___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 SS_16___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 SS_16___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.
Occupancy NEM_01		
Occupancy ratioNEM_01		
Occupancy error scale NEM_01		
Occupancy NEM_02		
Occupancy ratioNEM_02		
Occupancy error scale NEM_02		
Occupancy NEM_03		
Occupancy ratioNEM_03		
Occupancy error scale NEM_03		
Occupancy NEM_04		
Occupancy ratioNEM_04		
Occupancy error scale NEM_04		
Occupancy NEM_05		
Occupancy ratioNEM_05		
Occupancy error scale NEM_05		
Occupancy NEM_06		
Occupancy ratioNEM_06		
Occupancy error scale NEM_06		
Occupancy NEM_07		
Occupancy ratioNEM_07		
Occupancy error scale NEM_07		
Occupancy NEM_08		
Occupancy ratioNEM_08		
Occupancy error scale NEM_08		
Occupancy NEM_09		
Occupancy ratioNEM_09		
Occupancy error scale NEM_09		
Occupancy NEM_10		
Occupancy ratioNEM_10		
Occupancy error scale NEM_10		
Occupancy NEM_11		
Occupancy ratioNEM_11		
Occupancy error scale NEM_11		
Occupancy NEM_12		
Occupancy ratioNEM_12		
Occupancy error scale NEM_12		
Occupancy NEM_13		
Occupancy ratioNEM_13		
Occupancy error scale NEM_13		
Occupancy NEM_14		
Occupancy ratioNEM_14		
Occupancy error scale NEM_14		
Occupancy NEM_15		
Occupancy ratioNEM_15		
Occupancy error scale NEM_15		
Occupancy NEM_16		
Occupancy ratioNEM_16		
Occupancy error scale NEM_16		
Occupancy SS_01		

Occupancy ratioSS_01		
Occupancy error scale SS_01		
Occupancy SS_02		
Occupancy ratioSS_02		
Occupancy error scale SS_02		
Occupancy SS_03		
Occupancy ratioSS_03		
Occupancy error scale SS_03		
Occupancy SS_04		
Occupancy ratioSS_04		
Occupancy error scale SS_04		
Occupancy SS_05		
Occupancy ratioSS_05		
Occupancy error scale SS_05		
Occupancy SS_06		
Occupancy ratioSS_06		
Occupancy error scale SS_06		
Occupancy SS_07		
Occupancy ratioSS_07		
Occupancy error scale SS_07		
Occupancy SS_08		
Occupancy ratioSS_08		
Occupancy error scale SS_08		
Occupancy SS_09		
Occupancy ratioSS_09		
Occupancy error scale SS_09		
Occupancy SS_10		
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Occupancy SS_14		
Occupancy ratioSS_14		
Occupancy error scale SS_14		
Occupancy SS_15		
Occupancy ratioSS_15		
Occupancy error scale SS_15		
Occupancy SS_16		
Occupancy ratioSS_16		
Occupancy error scale SS_16		
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 NEM_01		
Score diff NEM_01		
PEP NEM_01		
Score NEM_01		
Localization prob NEM_02		
Score diff NEM_02		
PEP NEM_02		
Score NEM_02		
Localization prob NEM_03		
Score diff NEM_03		
PEP NEM_03		
Score NEM_03		
Localization prob NEM_04		
Score diff NEM_04		
PEP NEM_04		
Score NEM_04		
Localization prob NEM_05		
Score diff NEM_05		
PEP NEM_05		
Score NEM_05		
Localization prob NEM_06		
Score diff NEM_06		
PEP NEM_06		
Score NEM_06		
Localization prob NEM_07		
Score diff NEM_07		
PEP NEM_07		
Score NEM_07		
Localization prob NEM_08		
Score diff NEM_08		
PEP NEM_08		
Score NEM_08		
Localization prob NEM_09		
Score diff NEM_09		
PEP NEM_09		
Score NEM_09		
Localization prob NEM_10		
Score diff NEM_10		
PEP NEM_10		
Score NEM_10		
Localization prob NEM_11		
Score diff NEM_11		

PEP NEM_11		
Score NEM_11		
Localization prob NEM_12		
Score diff NEM_12		
PEP NEM_12		
Score NEM_12		
Localization prob NEM_13		
Score diff NEM_13		
PEP NEM_13		
Score NEM_13		
Localization prob NEM_14		
Score diff NEM_14		
PEP NEM_14		
Score NEM_14		
Localization prob NEM_15		
Score diff NEM_15		
PEP NEM_15		
Score NEM_15		
Localization prob NEM_16		
Score diff NEM_16		
PEP NEM_16		
Score NEM_16		
Localization prob SS_01		
Score diff SS_01		
PEP SS_01		
Score SS_01		
Localization prob SS_02		
Score diff SS_02		
PEP SS_02		
Score SS_02		
Localization prob SS_03		
Score diff SS_03		
PEP SS_03		
Score SS_03		
Localization prob SS_04		
Score diff SS_04		
PEP SS_04		
Score SS_04		
Localization prob SS_05		
Score diff SS_05		
PEP SS_05		
Score SS_05		
Localization prob SS_06		
Score diff SS_06		
PEP SS_06		
Score SS_06		
Localization prob SS_07		
Score diff SS_07		
PEP SS_07		
Score SS_07		
Localization prob SS_08		
Score diff SS_08		
PEP SS_08		
Score SS_08		
Localization prob SS_09		
Score diff SS_09		
PEP SS_09		
Score SS_09		
Localization prob SS_10		
Score diff SS_10		
PEP SS_10		
Score SS_10		
Localization prob SS_11		
Score diff SS_11		

PEP SS_11		
Score SS_11		
Localization prob SS_12		
Score diff SS_12		
PEP SS_12		
Score SS_12		
Localization prob SS_13		
Score diff SS_13		
PEP SS_13		
Score SS_13		
Localization prob SS_14		
Score diff SS_14		
PEP SS_14		
Score SS_14		
Localization prob SS_15		
Score diff SS_15		
PEP SS_15		
Score SS_15		
Localization prob SS_16		
Score diff SS_16		
PEP SS_16		
Score SS_16		
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 NEM_01		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_02		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_03		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_04		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_05		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_06		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_07		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_08		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_09		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_10		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_11		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_12		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_13		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_14		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_15		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_16		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SS_01		Indicates whether this experiment was identified by MS/MS or only by matching between runs.

Intensity SS_14		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 SS_15		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 SS_16		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 NEM_01		
Ratio mod/base NEM_02		
Ratio mod/base NEM_03		
Ratio mod/base NEM_04		
Ratio mod/base NEM_05		
Ratio mod/base NEM_06		
Ratio mod/base NEM_07		
Ratio mod/base NEM_08		
Ratio mod/base NEM_09		
Ratio mod/base NEM_10		
Ratio mod/base NEM_11		
Ratio mod/base NEM_12		
Ratio mod/base NEM_13		
Ratio mod/base NEM_14		
Ratio mod/base NEM_15		
Ratio mod/base NEM_16		
Ratio mod/base SS_01		
Ratio mod/base SS_02		
Ratio mod/base SS_03		
Ratio mod/base SS_04		
Ratio mod/base SS_05		
Ratio mod/base SS_06		
Ratio mod/base SS_07		
Ratio mod/base SS_08		
Ratio mod/base SS_09		
Ratio mod/base SS_10		
Ratio mod/base SS_11		
Ratio mod/base SS_12		
Ratio mod/base SS_13		
Ratio mod/base SS_14		
Ratio mod/base SS_15		
Ratio mod/base SS_16		
Intensity NEM_01___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 NEM_01___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 NEM_01___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 NEM_02___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 NEM_02___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 NEM_02___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 NEM_03___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 SS_15___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 SS_15___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 SS_16___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 SS_16___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 SS_16___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 NEM_01		Number of peptides (distinct peptide sequences) in experiment NEM_01
Peptides NEM_02		Number of peptides (distinct peptide sequences) in experiment NEM_02
Peptides NEM_03		Number of peptides (distinct peptide sequences) in experiment NEM_03
Peptides NEM_04		Number of peptides (distinct peptide sequences) in experiment NEM_04
Peptides NEM_05		Number of peptides (distinct peptide sequences) in experiment NEM_05
Peptides NEM_06		Number of peptides (distinct peptide sequences) in experiment NEM_06
Peptides NEM_07		Number of peptides (distinct peptide sequences) in experiment NEM_07
Peptides NEM_08		Number of peptides (distinct peptide sequences) in experiment NEM_08
Peptides NEM_09		Number of peptides (distinct peptide sequences) in experiment NEM_09
Peptides NEM_10		Number of peptides (distinct peptide sequences) in experiment NEM_10
Peptides NEM_11		Number of peptides (distinct peptide sequences) in experiment NEM_11
Peptides NEM_12		Number of peptides (distinct peptide sequences) in experiment NEM_12
Peptides NEM_13		Number of peptides (distinct peptide sequences) in experiment NEM_13
Peptides NEM_14		Number of peptides (distinct peptide sequences) in experiment NEM_14
Peptides NEM_15		Number of peptides (distinct peptide sequences) in experiment NEM_15
Peptides NEM_16		Number of peptides (distinct peptide sequences) in experiment NEM_16
Peptides SS_01		Number of peptides (distinct peptide sequences) in experiment SS_01
Peptides SS_02		Number of peptides (distinct peptide sequences) in experiment SS_02

Unique peptides SS_15		Number of unique peptides (distinct peptide sequences) in experiment SS_15
Unique peptides SS_16		Number of unique peptides (distinct peptide sequences) in experiment SS_16
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.
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 NEM_01		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_02		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_03		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_04		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_05		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_06		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_07		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_08		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_09		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_10		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_11		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_12		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_13		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_14		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_15		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type NEM_16		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SS_01		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SS_02		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SS_03		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SS_04		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SS_05		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SS_06		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SS_07		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SS_08		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SS_09		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SS_10		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SS_11		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type SS_12		Indicates whether this experiment was identified by MS/MS or only by matching between runs.

LFQ intensity NEM_11		
LFQ intensity NEM_12		
LFQ intensity NEM_13		
LFQ intensity NEM_14		
LFQ intensity NEM_15		
LFQ intensity NEM_16		
LFQ intensity SS_01		
LFQ intensity SS_02		
LFQ intensity SS_03		
LFQ intensity SS_04		
LFQ intensity SS_05		
LFQ intensity SS_06		
LFQ intensity SS_07		
LFQ intensity SS_08		
LFQ intensity SS_09		
LFQ intensity SS_10		
LFQ intensity SS_11		
LFQ intensity SS_12		
LFQ intensity SS_13		
LFQ intensity SS_14		
LFQ intensity SS_15		
LFQ intensity SS_16		
MS/MS count NEM_01		
MS/MS count NEM_02		
MS/MS count NEM_03		
MS/MS count NEM_04		
MS/MS count NEM_05		
MS/MS count NEM_06		
MS/MS count NEM_07		
MS/MS count NEM_08		
MS/MS count NEM_09		
MS/MS count NEM_10		
MS/MS count NEM_11		
MS/MS count NEM_12		
MS/MS count NEM_13		
MS/MS count NEM_14		
MS/MS count NEM_15		
MS/MS count NEM_16		
MS/MS count SS_01		
MS/MS count SS_02		
MS/MS count SS_03		
MS/MS count SS_04		
MS/MS count SS_05		
MS/MS count SS_06		
MS/MS count SS_07		
MS/MS count SS_08		
MS/MS count SS_09		
MS/MS count SS_10		
MS/MS count SS_11		
MS/MS count SS_12		
MS/MS count SS_13		
MS/MS count SS_14		
MS/MS count SS_15		
MS/MS count SS_16		
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.
NEM_free_CAA 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.
NEM_free_CAA 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.
Taxonomy IDs		Taxonomy identifiers.

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.
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.
Reverse		When marked with '+' this particular MS/MS scan was assigned to a decoy sequence.
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).
PEP		The posterior error probability of the identification (smaller is better).
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.
DP Mass Difference		Dependent peptide search: Mass Difference
DP Time Difference		Dependent peptide search: Time Difference
DP Score		Dependent peptide search: Score
DP PEP		Dependent peptide search: PEP
DP Positional Probability		Dependent peptide search: Positional Probability
DP Base Sequence		Dependent peptide search: Base Sequence
DP Probabilities		Dependent peptide search: Probabilities
DP AA		Dependent peptide search: AA
DP Base Raw File		Dependent peptide search: Base Scan Number
DP Base Scan Number		Dependent peptide search: Base Scan Number
DP Mod Scan Number		Dependent peptide search: Mod Scan Number
DP Decoy		Dependent peptide search: Decoy
DP Proteins		Dependent peptide search: Proteins
DP Cluster Index		Dependent peptide search: Cluster Index
DP Cluster Mass		Dependent peptide search: Cluster Mass
DP Cluster Mass SD		Dependent peptide search: Cluster Mass SD
DP Cluster Size Total		Dependent peptide search: Cluster Size Total
DP Cluster Size Forward		Dependent peptide search: Cluster Size Forward
DP Cluster Size Reverse		Dependent peptide search: Cluster Size Reverse
DP Modification		Dependent peptide search: Modification
DP Peptide Length Difference		Dependent peptide search: Peptide Length Difference
DP Ratio mod/base		Dependent peptide search: Ratio mod/base

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.
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.
Matched		When marked with '+' this particular MS/MS scan was retrieved by matching between runs.
Reverse		When marked with '+' this particular MS/MS scan was assigned to a decoy sequence.
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).
PEP		The posterior error probability of the identification (smaller is better).
Experiment		
Reporter PIF		
Reporter fraction		
DP mass difference		This dependent peptide's mass difference to the associated identified peptide.
DP time difference		This dependent peptide's time difference to the associated identified peptide.
DP score		The andromeda identification score.
DP PEP		Posterior Error Probability of the identification. This value essentially operates as a p-value, where smaller is more significant.
DP positional probability		
DP base sequence		
DP probabilities		
DP AA		
DP base raw file		
DP base scan number		
DP mod scan number		
DP decoy		
DP proteins		
DP cluster index		
DP cluster mass		
DP cluster mass SD		
DP cluster size total		
DP cluster size forward		
DP cluster size reverse		
DP modification		Post-translational modifications contained within the sequence. When no modifications exist, this is set to 'unmodified'.
DP peptide length difference		
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 (AspN)		Number of missed enzymatic cleavages.
Missed cleavages (AspN;GluC_phos)		Number of missed enzymatic cleavages.
Missed cleavages (Chymotrypsin+)		Number of missed enzymatic cleavages.
Missed cleavages (Trypsin/P)		Number of missed enzymatic cleavages.
Missed cleavages (Trypsin/P;AspN)		Number of missed enzymatic cleavages.
Missed cleavages (GluC_phos)		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 ('_').
NEM_free_CAA Probabilities		Sequence representation of the peptide including PTM positioning probabilities ([0..1], where 1 is best match) for 'NEM_free_CAA'.
Oxidation (M) Probabilities		Sequence representation of the peptide including PTM positioning probabilities ([0..1], where 1 is best match) for 'Oxidation (M)'.
NEM_free_CAA Score diffs		
Oxidation (M) Score diffs		
Acetyl (Protein N-term)		
NEM_free_CAA		
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'.
NEM_free_CAA site IDs		Identifier of the associated entry stored in the file 'NEM_free_CAASites.txt'.
Oxidation (M) site IDs		Identifier of the associated entry stored in the file 'Oxidation (M)Sites.txt'.

Dependent peptides

Name	Separator	Description
Base peptide sequence		Base peptide sequence. Entries for the dependent peptides table get aggregated if they have the same base peptide sequence, modification and cluster index!
Modification		Modification. Entries for the dependent peptides table get aggregated if they have the same base peptide sequence, modification and cluster index!
Cluster index		Cluster index Entries for the dependent peptides table get aggregated if they have the same base peptide sequence, modification and cluster index!
Cluster mass		Cluster mass
Cluster mass SD		Cluster Mass SD
Cluster size total		Cluster Size Total
Cluster size forward		Cluster Size Forward
Cluster size reverse		Cluster Size Reverse
Base peptide raw file		This column contains the names of raw files that contained the original unmodified base peptide spectrum which were used to search for additional dependent peptides.
Matches in Raw files		This column represents all the raw files where the dependent Peptide could be found.
Type		The type of detection for the dependent peptide. Multi – A labeling multiplet was detected. Iso – An isotope pattern was detected.
Localization probability		Base peptide sequence combined with the localization probability of possible candidates for the modification
Max Probability		The column contains the highest probability form an aminoacid candidate.
Posterior error probability		Posterior error probability
Aminoacid localizations		This contains all the possible amino acid candidates for the modification as well as information if they could be n or c - Terminal.
Feature Ids		The Feature Id can be used with the according raw file to trace a dependent peptide entry back in other tables. E.g: AllPeptides or MatchedFeatures - tables.
Found by		Information about how Identification and Quantification was acquired. Regular dependent peptide search: base raw file and matched raw file are equal. Dependent base peptide aggregation search: an other raw file was utilized to identify then the one the dep. peptide is in. Match unidentified features: an unidentified feature was detected by match unidentified features but not dependent peptide search.(dependent peptides are unidentified features)
Amount found by regular search		Information about how often specific Identification and Quantification was acquired.
Amount found by base peptide aggregation		Information about how often specific Identification and Quantification was acquired.
Amount found by match unidentified features		Information about how often specific Identification and Quantification was acquired.
AllPeptides Ids		This represents the index in the AllPeptides table of a dependent peptide entry. It's an easier way of finding the dependent peptide entry within the table than with the FeatureId!
Score		
Mass difference		Mass Difference
Time difference		Time Difference
Peptide Length Difference		Peptide Length Difference
Protein IDs		
Modification intensities		
Modification scan numbers		The modification scan numbers can be used to search a dependent peptide entry in msmsScans table.
Base intensity Exp: NEM_01		This column contains the base intensity for the experiment. If there are multiple dependent peptides found in this raw file than their intensities will get aggregated.
Base intensity Exp: NEM_02		This column contains the base intensity for the experiment. If there are multiple dependent peptides found in this raw file than their intensities will get aggregated.
Base intensity Exp: NEM_03		This column contains the base intensity for the experiment. If there are multiple dependent peptides found in this raw file than their intensities will get aggregated.

Ratio mod/base intensity Exp: SS_13		This column contains the ratio between modification and base intensity for the specific experiment.
Ratio mod/base intensity Exp: SS_14		This column contains the ratio between modification and base intensity for the specific experiment.
Ratio mod/base intensity Exp: SS_15		This column contains the ratio between modification and base intensity for the specific experiment.
Ratio mod/base intensity Exp: SS_16		This column contains the ratio between modification and base intensity for the specific experiment.