

# 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.
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 ('_').
Oxidation (M) Probabilities		Sequence representation of the peptide including PTM positioning probabilities ([0..1], where 1 is best match) for 'Oxidation (M)'.
Phospho (STY) Probabilities		Sequence representation of the peptide including PTM positioning probabilities ([0..1], where 1 is best match) for 'Phospho (STY)'.
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.
Phospho (STY) 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)'.
Oxidation (M)		The number of occurrences of the modification 'Oxidation (M)'.
Phospho (STY)		The number of occurrences of the modification 'Phospho (STY)'.
Missed cleavages		Number of missed enzymatic cleavages.
Proteins		The identifiers of the proteins this particular peptide is associated with.
Leading proteins		The identifiers of the proteins in the proteinGroups file, with this protein as best match, this particular peptide is associated with. When multiple matches are found here, the best scoring protein can be found in the 'Leading Razor Protein' column.
Leading razor protein		The identifier of the best scoring protein, from the proteinGroups file this, this peptide is associated to.
Type		The type of the feature. MSMS – MS/MS 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.
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.
Resolution		The resolution of precursor ion measured in Full Width at Half Maximum (FWHM).
Uncalibrated - Calibrated m/z [ppm]		The difference between the uncalibrated and recalibrated mass-over-charge value of the precursor ion measured in parts-per-million. This gives an indication of the mass drift in the original data, which was automatically corrected by MaxQuant.
Uncalibrated - Calibrated m/z [Da]		The difference between the uncalibrated and recalibrated mass-over-charge value of the precursor ion measured in parts-per-million. This gives an indication of the mass drift in the original data, which was automatically corrected by MaxQuant.

Mass Error [ppm]		Mass error of the recalibrated mass-over-charge value of the precursor ion in comparison to the predicted monoisotopic mass of the identified peptide sequence in parts per million.
Mass Error [Da]		Mass error of the recalibrated mass-over-charge value of the precursor ion in comparison to the predicted monoisotopic mass of the identified peptide sequence in milli-Dalton.
Uncalibrated Mass Error [ppm]		Mass error of the uncalibrated mass-over-charge value of the precursor ion in comparison to the predicted monoisotopic mass of the identified peptide sequence.  Note: This column can contain missing values (denoted as NaN).
Uncalibrated Mass Error [Da]		Mass error of the uncalibrated mass-over-charge value of the precursor ion in comparison to the predicted monoisotopic mass of the identified peptide sequence.  Note: This column can contain missing values (denoted as NaN).
Max intensity m/z 0		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Retention time		The uncalibrated retention time in minutes in the elution profile of the precursor ion.
Retention length		The total retention time of the peak (last timepoint – first timepoint).
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'. This number is independent of the times the AA sequence has been identified through (other) modifications (e.g. heavy label, oxidation, etc.), about which information can be found in the columns 'Labeling State' and 'Modification'.
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 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'.
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'.
AIF MS/MS IDs		Identifier(s) of the associated All Ion Fragmentation MS/MS summary(s) stored in the file 'aifMsms.txt'.
Oxidation (M) site IDs		Identifier(s) of the modification summary stored in the file 'Oxidation (M)Sites.txt'.
Phospho (STY) site IDs		Identifier(s) of the modification summary stored in the file 'Phospho (STY)Sites.txt'.

# Peptides

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

Name	Separator	Description
Sequence		The amino acid sequence of the identified peptide.
N-term cleavage window		Sequence window from -8 to 8 around the N-terminal cleavage site of this peptide.
C-term cleavage window		Sequence window from -8 to 8 around the C-terminal cleavage site of this peptide.
Amino acid before		The amino acid in the protein sequence before the peptide.
First amino acid		The amino acid in the first position of the peptide sequence.
Second amino acid		The amino acid in the first position of the peptide sequence.
Second last amino acid		The amino acid in the last position of the peptide sequence.
Last amino acid		The amino acid in the last position of the peptide sequence.
Amino acid after		The amino acid in the protein sequence after the peptide.
A Count		The number of instances of the 'A' amino acid contained within the sequence.
R Count		The number of instances of the 'R' amino acid contained within the sequence.
N Count		The number of instances of the 'N' amino acid contained within the sequence.
D Count		The number of instances of the 'D' amino acid contained within the sequence.
C Count		The number of instances of the 'C' amino acid contained within the sequence.
Q Count		The number of instances of the 'Q' amino acid contained within the sequence.
E Count		The number of instances of the 'E' amino acid contained within the sequence.
G Count		The number of instances of the 'G' amino acid contained within the sequence.
H Count		The number of instances of the 'H' amino acid contained within the sequence.
I Count		The number of instances of the 'I' amino acid contained within the sequence.
L Count		The number of instances of the 'L' amino acid contained within the sequence.
K Count		The number of instances of the 'K' amino acid contained within the sequence.
M Count		The number of instances of the 'M' amino acid contained within the sequence.
F Count		The number of instances of the 'F' amino acid contained within the sequence.
P Count		The number of instances of the 'P' amino acid contained within the sequence.
S Count		The number of instances of the 'S' amino acid contained within the sequence.
T Count		The number of instances of the 'T' amino acid contained within the sequence.
W Count		The number of instances of the 'W' amino acid contained within the sequence.
Y Count		The number of instances of the 'Y' amino acid contained within the sequence.
V Count		The number of instances of the 'V' amino acid contained within the sequence.
U Count		The number of instances of the 'U' amino acid contained within the sequence.
O Count		The number of instances of the 'O' amino acid contained within the sequence.
Length		The length of the sequence stored in the column "Sequence".
Missed cleavages		Number of missed enzymatic cleavages.
Mass		Monoisotopic mass of the peptide.
Proteins		Identifiers of proteins this peptide is associated with.
Leading razor protein		Identifiers of the best scoring protein this peptide is associated with.
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 Apubscrawl_Cerulenin_Ub		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Apubscrawl_Cerulenin_UbP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Apubscrawl_Cerulenin_WCL		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Apubscrawl_Cerulenin_WCLP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Apubscrawl_Swe1KO_Ub		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Apubscrawl_Swe1KO_UbP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Apubscrawl_Swe1KO_WCL		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Apubscrawl_Swe1KO_WCLP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Control_Ub		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Control_UbP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Control_WCL		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Control_WCLP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type EtOH_Kin3KO_Ub		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type EtOH_Kin3KO_UbP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type EtOH_Kin3KO_WCL		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type EtOH_Kin3KO_WCLP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type EtOH_menadione_Ub		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type EtOH_menadione_UbP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type EtOH_menadione_WCL		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type EtOH_menadione_WCLP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Onion_Atg1KO_Ub		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Onion_Atg1KO_UbP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Onion_Atg1KO_WCL		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Onion_Atg1KO_WCLP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Onion_rapamycin_Ub		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Onion_rapamycin_UbP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Onion_rapamycin_WCL		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Onion_rapamycin_WCLP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Pynd_5FC_Ub		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Pynd_5FC_UbP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Pynd_5FC_WCL		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Pynd_5FC_WCLP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Pynd_AikKO_Ub		Indicates whether this experiment was identified by MS/MS or only by matching between runs.

Identification type Pynd_AlkKO_UbP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Pynd_AlkKO_WCL		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Pynd_AlkKO_WCLP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Shmoo_CaCl2_Ub		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Shmoo_CaCl2_WCL		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Shmoo_Cmk1KO_Ub		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Shmoo_Cmk1KO_UbP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Shmoo_Cmk1KO_WCL		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Shmoo_Cmk1KO_WCLP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Whangee_Tpk1KO_Ub		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Whangee_Tpk1KO_UbP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Whangee_Tpk1KO_WCL		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Whangee_Tpk1KO_WCLP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Whangee_tunicamycin_Ub		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Whangee_tunicamycin_UbP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Whangee_tunicamycin_WCL		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Whangee_tunicamycin_WCLP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Experiment Apubscrawl_Cerulenin_Ub		Number of evidence entries for this 'Experiment'.
Experiment Apubscrawl_Cerulenin_UbP		Number of evidence entries for this 'Experiment'.
Experiment Apubscrawl_Cerulenin_WCL		Number of evidence entries for this 'Experiment'.
Experiment Apubscrawl_Cerulenin_WCLP		Number of evidence entries for this 'Experiment'.
Experiment Apubscrawl_Swe1KO_Ub		Number of evidence entries for this 'Experiment'.
Experiment Apubscrawl_Swe1KO_UbP		Number of evidence entries for this 'Experiment'.
Experiment Apubscrawl_Swe1KO_WCL		Number of evidence entries for this 'Experiment'.
Experiment Apubscrawl_Swe1KO_WCLP		Number of evidence entries for this 'Experiment'.
Experiment Control_Ub		Number of evidence entries for this 'Experiment'.
Experiment Control_UbP		Number of evidence entries for this 'Experiment'.
Experiment Control_WCL		Number of evidence entries for this 'Experiment'.
Experiment Control_WCLP		Number of evidence entries for this 'Experiment'.
Experiment EtOH_Kin3KO_Ub		Number of evidence entries for this 'Experiment'.
Experiment EtOH_Kin3KO_UbP		Number of evidence entries for this 'Experiment'.
Experiment EtOH_Kin3KO_WCL		Number of evidence entries for this 'Experiment'.
Experiment EtOH_Kin3KO_WCLP		Number of evidence entries for this 'Experiment'.
Experiment EtOH_menadione_Ub		Number of evidence entries for this 'Experiment'.
Experiment EtOH_menadione_UbP		Number of evidence entries for this 'Experiment'.
Experiment EtOH_menadione_WCL		Number of evidence entries for this 'Experiment'.
Experiment EtOH_menadione_WCLP		Number of evidence entries for this 'Experiment'.
Experiment Onion_Atg1KO_Ub		Number of evidence entries for this 'Experiment'.
Experiment Onion_Atg1KO_UbP		Number of evidence entries for this 'Experiment'.
Experiment Onion_Atg1KO_WCL		Number of evidence entries for this 'Experiment'.
Experiment Onion_Atg1KO_WCLP		Number of evidence entries for this 'Experiment'.
Experiment Onion_rapamycin_Ub		Number of evidence entries for this 'Experiment'.
Experiment Onion_rapamycin_UbP		Number of evidence entries for this 'Experiment'.
Experiment Onion_rapamycin_WCL		Number of evidence entries for this 'Experiment'.
Experiment Onion_rapamycin_WCLP		Number of evidence entries for this 'Experiment'.
Experiment Pynd_5FC_Ub		Number of evidence entries for this 'Experiment'.



Experiment Pynd_5FC_UbP		Number of evidence entries for this 'Experiment'.
Experiment Pynd_5FC_WCL		Number of evidence entries for this 'Experiment'.
Experiment Pynd_5FC_WCLP		Number of evidence entries for this 'Experiment'.
Experiment Pynd_AlkKO_Ub		Number of evidence entries for this 'Experiment'.
Experiment Pynd_AlkKO_UbP		Number of evidence entries for this 'Experiment'.
Experiment Pynd_AlkKO_WCL		Number of evidence entries for this 'Experiment'.
Experiment Pynd_AlkKO_WCLP		Number of evidence entries for this 'Experiment'.
Experiment Shmoo_CaCl2_Ub		Number of evidence entries for this 'Experiment'.
Experiment Shmoo_CaCl2_WCL		Number of evidence entries for this 'Experiment'.
Experiment Shmoo_Cmk1KO_Ub		Number of evidence entries for this 'Experiment'.
Experiment Shmoo_Cmk1KO_UbP		Number of evidence entries for this 'Experiment'.
Experiment Shmoo_Cmk1KO_WCL		Number of evidence entries for this 'Experiment'.
Experiment Shmoo_Cmk1KO_WCLP		Number of evidence entries for this 'Experiment'.
Experiment Whangee_Tpk1KO_Ub		Number of evidence entries for this 'Experiment'.
Experiment Whangee_Tpk1KO_UbP		Number of evidence entries for this 'Experiment'.
Experiment Whangee_Tpk1KO_WCL		Number of evidence entries for this 'Experiment'.
Experiment Whangee_Tpk1KO_WCLP		Number of evidence entries for this 'Experiment'.
Experiment Whangee_tunicamycin_Ub		Number of evidence entries for this 'Experiment'.
Experiment Whangee_tunicamycin_UbP		Number of evidence entries for this 'Experiment'.
Experiment Whangee_tunicamycin_WCL		Number of evidence entries for this 'Experiment'.
Experiment Whangee_tunicamycin_WCLP		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 Apubscrawl_Cerulenin_Ub		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 Apubscrawl_Cerulenin_UbP		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 Apubscrawl_Cerulenin_WCL		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 Apubscrawl_Cerulenin_WCLP		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 Apubscrawl_Swe1KO_Ub		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 Apubscrawl_Swe1KO_UbP		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 Apubscrawl_Swe1KO_WCL		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 Apubscrawl_Swe1KO_WCLP		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 Control_Ub		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 Control_UbP		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 Control_WCL		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.

[illegible]

Intensity Pynd_AlkKO_Ub		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 Pynd_AlkKO_UbP		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 Pynd_AlkKO_WCL		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 Pynd_AlkKO_WCLP		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 Shmoo_CaCl2_Ub		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 Shmoo_CaCl2_WCL		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 Shmoo_Cmk1KO_Ub		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 Shmoo_Cmk1KO_UbP		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 Shmoo_Cmk1KO_WCL		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 Shmoo_Cmk1KO_WCLP		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 Whangee_Tpk1KO_Ub		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 Whangee_Tpk1KO_UbP		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 Whangee_Tpk1KO_WCL		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 Whangee_Tpk1KO_WCLP		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 Whangee_tunicamycin_Ub		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 Whangee_tunicamycin_UbP		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 Whangee_tunicamycin_WCL		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 Whangee_tunicamycin_WCLP		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 evidences 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.
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.
Phospho (STY) site IDs		Identifier(s) for site(s) associated with the protein group, which show(s) evidence of the modification, referenced against the appropriate modification site file.
MS/MS Count		

# 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.
Oxidation (M)		Number of Oxidation (M) on this peptide.
Phospho (STY)		Number of Phospho (STY) on this peptide.
Missed cleavages		Number of missed enzymatic cleavages.
Identification type Apubscrawl_Cerulenin_Ub		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Apubscrawl_Cerulenin_UbP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Apubscrawl_Cerulenin_WCL		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Apubscrawl_Cerulenin_WCLP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Apubscrawl_Swe1KO_Ub		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Apubscrawl_Swe1KO_UbP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Apubscrawl_Swe1KO_WCL		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Apubscrawl_Swe1KO_WCLP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Control_Ub		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Control_UbP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Control_WCL		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Control_WCLP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type EtOH_Kin3KO_Ub		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type EtOH_Kin3KO_UbP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type EtOH_Kin3KO_WCL		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type EtOH_Kin3KO_WCLP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type EtOH_menadione_Ub		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type EtOH_menadione_UbP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type EtOH_menadione_WCL		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type EtOH_menadione_WCLP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Onion_At1KO_Ub		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Onion_At1KO_UbP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Onion_At1KO_WCL		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Onion_At1KO_WCLP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Onion_rapamycin_Ub		Indicates whether this experiment was identified by MS/MS or only by matching between runs.

Identification type Onion_rapamycin_UbP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Onion_rapamycin_WCL		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Onion_rapamycin_WCLP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Pynd_5FC_Ub		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Pynd_5FC_UbP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Pynd_5FC_WCL		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Pynd_5FC_WCLP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Pynd_AlkkO_Ub		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Pynd_AlkkO_UbP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Pynd_AlkkO_WCL		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Pynd_AlkkO_WCLP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Shmoo_CaCl2_Ub		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Shmoo_CaCl2_WCL		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Shmoo_Cmk1KO_Ub		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Shmoo_Cmk1KO_UbP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Shmoo_Cmk1KO_WCL		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Shmoo_Cmk1KO_WCLP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Whangee_Tpk1KO_Ub		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Whangee_Tpk1KO_UbP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Whangee_Tpk1KO_WCL		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Whangee_Tpk1KO_WCLP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Whangee_tunicamycin_Ub		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Whangee_tunicamycin_UbP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Whangee_tunicamycin_WCL		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Whangee_tunicamycin_WCLP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Experiment Apubscrawl_Cerulenin_Ub		Number of evidence entries for this 'Experiment'.
Experiment Apubscrawl_Cerulenin_UbP		Number of evidence entries for this 'Experiment'.
Experiment Apubscrawl_Cerulenin_WCL		Number of evidence entries for this 'Experiment'.
Experiment Apubscrawl_Cerulenin_WCLP		Number of evidence entries for this 'Experiment'.
Experiment Apubscrawl_Swe1KO_Ub		Number of evidence entries for this 'Experiment'.
Experiment Apubscrawl_Swe1KO_UbP		Number of evidence entries for this 'Experiment'.
Experiment Apubscrawl_Swe1KO_WCL		Number of evidence entries for this 'Experiment'.
Experiment Apubscrawl_Swe1KO_WCLP		Number of evidence entries for this 'Experiment'.
Experiment Control_Ub		Number of evidence entries for this 'Experiment'.
Experiment Control_UbP		Number of evidence entries for this 'Experiment'.
Experiment Control_WCL		Number of evidence entries for this 'Experiment'.
Experiment Control_WCLP		Number of evidence entries for this 'Experiment'.
Experiment EtOH_Kin3KO_Ub		Number of evidence entries for this 'Experiment'.
Experiment EtOH_Kin3KO_UbP		Number of evidence entries for this 'Experiment'.
Experiment EtOH_Kin3KO_WCL		Number of evidence entries for this 'Experiment'.
Experiment EtOH_Kin3KO_WCLP		Number of evidence entries for this 'Experiment'.
Experiment EtOH_menadione_Ub		Number of evidence entries for this 'Experiment'.

Experiment EtOH_menadione_UbP		Number of evidence entries for this 'Experiment'.
Experiment EtOH_menadione_WCL		Number of evidence entries for this 'Experiment'.
Experiment EtOH_menadione_WCLP		Number of evidence entries for this 'Experiment'.
Experiment Onion_At1KO_Ub		Number of evidence entries for this 'Experiment'.
Experiment Onion_At1KO_UbP		Number of evidence entries for this 'Experiment'.
Experiment Onion_At1KO_WCL		Number of evidence entries for this 'Experiment'.
Experiment Onion_At1KO_WCLP		Number of evidence entries for this 'Experiment'.
Experiment Onion_rapamycin_Ub		Number of evidence entries for this 'Experiment'.
Experiment Onion_rapamycin_UbP		Number of evidence entries for this 'Experiment'.
Experiment Onion_rapamycin_WCL		Number of evidence entries for this 'Experiment'.
Experiment Onion_rapamycin_WCLP		Number of evidence entries for this 'Experiment'.
Experiment Pynd_5FC_Ub		Number of evidence entries for this 'Experiment'.
Experiment Pynd_5FC_UbP		Number of evidence entries for this 'Experiment'.
Experiment Pynd_5FC_WCL		Number of evidence entries for this 'Experiment'.
Experiment Pynd_5FC_WCLP		Number of evidence entries for this 'Experiment'.
Experiment Pynd_AlkKO_Ub		Number of evidence entries for this 'Experiment'.
Experiment Pynd_AlkKO_UbP		Number of evidence entries for this 'Experiment'.
Experiment Pynd_AlkKO_WCL		Number of evidence entries for this 'Experiment'.
Experiment Pynd_AlkKO_WCLP		Number of evidence entries for this 'Experiment'.
Experiment Shmoo_CaCl2_Ub		Number of evidence entries for this 'Experiment'.
Experiment Shmoo_CaCl2_WCL		Number of evidence entries for this 'Experiment'.
Experiment Shmoo_Cmk1KO_Ub		Number of evidence entries for this 'Experiment'.
Experiment Shmoo_Cmk1KO_UbP		Number of evidence entries for this 'Experiment'.
Experiment Shmoo_Cmk1KO_WCL		Number of evidence entries for this 'Experiment'.
Experiment Shmoo_Cmk1KO_WCLP		Number of evidence entries for this 'Experiment'.
Experiment Whangee_Tpk1KO_Ub		Number of evidence entries for this 'Experiment'.
Experiment Whangee_Tpk1KO_UbP		Number of evidence entries for this 'Experiment'.
Experiment Whangee_Tpk1KO_WCL		Number of evidence entries for this 'Experiment'.
Experiment Whangee_Tpk1KO_WCLP		Number of evidence entries for this 'Experiment'.
Experiment Whangee_tunicamycin_Ub		Number of evidence entries for this 'Experiment'.
Experiment Whangee_tunicamycin_UbP		Number of evidence entries for this 'Experiment'.
Experiment Whangee_tunicamycin_WCL		Number of evidence entries for this 'Experiment'.
Experiment Whangee_tunicamycin_WCLP		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		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 Apubscrawl_Cerulenin_Ub		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 Apubscrawl_Cerulenin_UbP		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.

[illegible]



[illegible]

Intensity Whangee_Tpk1KO_WCL		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 Whangee_Tpk1KO_WCLP		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 Whangee_tunicamycin_Ub		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 Whangee_tunicamycin_UbP		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 Whangee_tunicamycin_WCL		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 Whangee_tunicamycin_WCLP		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.
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 evidences 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.
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.
Phospho (STY) 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		

# 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 Apubscrawl_Cerulenin_Ub		
Score diff Apubscrawl_Cerulenin_Ub		
PEP Apubscrawl_Cerulenin_Ub		
Score Apubscrawl_Cerulenin_Ub		
Localization prob Apubscrawl_Cerulenin_UbP		
Score diff Apubscrawl_Cerulenin_UbP		
PEP Apubscrawl_Cerulenin_UbP		
Score Apubscrawl_Cerulenin_UbP		
Localization prob Apubscrawl_Cerulenin_WCL		
Score diff Apubscrawl_Cerulenin_WCL		
PEP Apubscrawl_Cerulenin_WCL		
Score Apubscrawl_Cerulenin_WCL		
Localization prob Apubscrawl_Cerulenin_WCLP		
Score diff Apubscrawl_Cerulenin_WCLP		
PEP Apubscrawl_Cerulenin_WCLP		
Score Apubscrawl_Cerulenin_WCLP		
Localization prob Apubscrawl_Swe1KO_Ub		
Score diff Apubscrawl_Swe1KO_Ub		
PEP Apubscrawl_Swe1KO_Ub		
Score Apubscrawl_Swe1KO_Ub		
Localization prob Apubscrawl_Swe1KO_UbP		
Score diff Apubscrawl_Swe1KO_UbP		
PEP Apubscrawl_Swe1KO_UbP		
Score Apubscrawl_Swe1KO_UbP		
Localization prob Apubscrawl_Swe1KO_WCL		
Score diff Apubscrawl_Swe1KO_WCL		
PEP Apubscrawl_Swe1KO_WCL		
Score Apubscrawl_Swe1KO_WCL		
Localization prob Apubscrawl_Swe1KO_WCLP		
Score diff Apubscrawl_Swe1KO_WCLP		
PEP Apubscrawl_Swe1KO_WCLP		
Score Apubscrawl_Swe1KO_WCLP		

Localization prob Control_Ub		
Score diff Control_Ub		
PEP Control_Ub		
Score Control_Ub		
Localization prob Control_UbP		
Score diff Control_UbP		
PEP Control_UbP		
Score Control_UbP		
Localization prob Control_WCL		
Score diff Control_WCL		
PEP Control_WCL		
Score Control_WCL		
Localization prob Control_WCLP		
Score diff Control_WCLP		
PEP Control_WCLP		
Score Control_WCLP		
Localization prob EtOH_Kin3KO_Ub		
Score diff EtOH_Kin3KO_Ub		
PEP EtOH_Kin3KO_Ub		
Score EtOH_Kin3KO_Ub		
Localization prob EtOH_Kin3KO_UbP		
Score diff EtOH_Kin3KO_UbP		
PEP EtOH_Kin3KO_UbP		
Score EtOH_Kin3KO_UbP		
Localization prob EtOH_Kin3KO_WCL		
Score diff EtOH_Kin3KO_WCL		
PEP EtOH_Kin3KO_WCL		
Score EtOH_Kin3KO_WCL		
Localization prob EtOH_Kin3KO_WCLP		
Score diff EtOH_Kin3KO_WCLP		
PEP EtOH_Kin3KO_WCLP		
Score EtOH_Kin3KO_WCLP		
Localization prob EtOH_menadione_Ub		
Score diff EtOH_menadione_Ub		
PEP EtOH_menadione_Ub		
Score EtOH_menadione_Ub		
Localization prob EtOH_menadione_UbP		
Score diff EtOH_menadione_UbP		
PEP EtOH_menadione_UbP		
Score EtOH_menadione_UbP		
Localization prob EtOH_menadione_WCL		
Score diff EtOH_menadione_WCL		
PEP EtOH_menadione_WCL		
Score EtOH_menadione_WCL		
Localization prob EtOH_menadione_WCLP		
Score diff EtOH_menadione_WCLP		
PEP EtOH_menadione_WCLP		
Score EtOH_menadione_WCLP		
Localization prob Onion_Atg1KO_Ub		
Score diff Onion_Atg1KO_Ub		
PEP Onion_Atg1KO_Ub		
Score Onion_Atg1KO_Ub		
Localization prob Onion_Atg1KO_UbP		
Score diff Onion_Atg1KO_UbP		
PEP Onion_Atg1KO_UbP		
Score Onion_Atg1KO_UbP		
Localization prob Onion_Atg1KO_WCL		

Score diff Onion_Atg1KO_WCL		
PEP Onion_Atg1KO_WCL		
Score Onion_Atg1KO_WCL		
Localization prob Onion_Atg1KO_WCLP		
Score diff Onion_Atg1KO_WCLP		
PEP Onion_Atg1KO_WCLP		
Score Onion_Atg1KO_WCLP		
Localization prob Onion_rapamycin_Ub		
Score diff Onion_rapamycin_Ub		
PEP Onion_rapamycin_Ub		
Score Onion_rapamycin_Ub		
Localization prob Onion_rapamycin_UbP		
Score diff Onion_rapamycin_UbP		
PEP Onion_rapamycin_UbP		
Score Onion_rapamycin_UbP		
Localization prob Onion_rapamycin_WCL		
Score diff Onion_rapamycin_WCL		
PEP Onion_rapamycin_WCL		
Score Onion_rapamycin_WCL		
Localization prob Onion_rapamycin_WCLP		
Score diff Onion_rapamycin_WCLP		
PEP Onion_rapamycin_WCLP		
Score Onion_rapamycin_WCLP		
Localization prob Pynd_5FC_Ub		
Score diff Pynd_5FC_Ub		
PEP Pynd_5FC_Ub		
Score Pynd_5FC_Ub		
Localization prob Pynd_5FC_UbP		
Score diff Pynd_5FC_UbP		
PEP Pynd_5FC_UbP		
Score Pynd_5FC_UbP		
Localization prob Pynd_5FC_WCL		
Score diff Pynd_5FC_WCL		
PEP Pynd_5FC_WCL		
Score Pynd_5FC_WCL		
Localization prob Pynd_5FC_WCLP		
Score diff Pynd_5FC_WCLP		
PEP Pynd_5FC_WCLP		
Score Pynd_5FC_WCLP		
Localization prob Pynd_AlkKO_Ub		
Score diff Pynd_AlkKO_Ub		
PEP Pynd_AlkKO_Ub		
Score Pynd_AlkKO_Ub		
Localization prob Pynd_AlkKO_UbP		
Score diff Pynd_AlkKO_UbP		
PEP Pynd_AlkKO_UbP		
Score Pynd_AlkKO_UbP		
Localization prob Pynd_AlkKO_WCL		
Score diff Pynd_AlkKO_WCL		
PEP Pynd_AlkKO_WCL		
Score Pynd_AlkKO_WCL		
Localization prob Pynd_AlkKO_WCLP		
Score diff Pynd_AlkKO_WCLP		
PEP Pynd_AlkKO_WCLP		
Score Pynd_AlkKO_WCLP		
Localization prob Shmoo_CaCl2_Ub		
Score diff Shmoo_CaCl2_Ub		
PEP Shmoo_CaCl2_Ub		

Score Shmoo_CaCl2_Ub		
Localization prob Shmoo_CaCl2_WCL		
Score diff Shmoo_CaCl2_WCL		
PEP Shmoo_CaCl2_WCL		
Score Shmoo_CaCl2_WCL		
Localization prob Shmoo_Cmk1KO_Ub		
Score diff Shmoo_Cmk1KO_Ub		
PEP Shmoo_Cmk1KO_Ub		
Score Shmoo_Cmk1KO_Ub		
Localization prob Shmoo_Cmk1KO_UbP		
Score diff Shmoo_Cmk1KO_UbP		
PEP Shmoo_Cmk1KO_UbP		
Score Shmoo_Cmk1KO_UbP		
Localization prob Shmoo_Cmk1KO_WCL		
Score diff Shmoo_Cmk1KO_WCL		
PEP Shmoo_Cmk1KO_WCL		
Score Shmoo_Cmk1KO_WCL		
Localization prob Shmoo_Cmk1KO_WCLP		
Score diff Shmoo_Cmk1KO_WCLP		
PEP Shmoo_Cmk1KO_WCLP		
Score Shmoo_Cmk1KO_WCLP		
Localization prob Whangee_Tpk1KO_Ub		
Score diff Whangee_Tpk1KO_Ub		
PEP Whangee_Tpk1KO_Ub		
Score Whangee_Tpk1KO_Ub		
Localization prob Whangee_Tpk1KO_UbP		
Score diff Whangee_Tpk1KO_UbP		
PEP Whangee_Tpk1KO_UbP		
Score Whangee_Tpk1KO_UbP		
Localization prob Whangee_Tpk1KO_WCL		
Score diff Whangee_Tpk1KO_WCL		
PEP Whangee_Tpk1KO_WCL		
Score Whangee_Tpk1KO_WCL		
Localization prob Whangee_Tpk1KO_WCLP		
Score diff Whangee_Tpk1KO_WCLP		
PEP Whangee_Tpk1KO_WCLP		
Score Whangee_Tpk1KO_WCLP		
Localization prob Whangee_tunicamycin_Ub		
Score diff Whangee_tunicamycin_Ub		
PEP Whangee_tunicamycin_Ub		
Score Whangee_tunicamycin_Ub		
Localization prob Whangee_tunicamycin_UbP		
Score diff Whangee_tunicamycin_UbP		
PEP Whangee_tunicamycin_UbP		
Score Whangee_tunicamycin_UbP		
Localization prob Whangee_tunicamycin_WCL		
Score diff Whangee_tunicamycin_WCL		
PEP Whangee_tunicamycin_WCL		
Score Whangee_tunicamycin_WCL		
Localization prob Whangee_tunicamycin_WCLP		
Score diff Whangee_tunicamycin_WCLP		
PEP Whangee_tunicamycin_WCLP		

Score		
Whangee_tunicamycin_WCLP		
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 Apubscrawl_Cerulenin_Ub		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Apubscrawl_Cerulenin_UbP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Apubscrawl_Cerulenin_WCL		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Apubscrawl_Cerulenin_WCLP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Apubscrawl_Swe1KO_Ub		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Apubscrawl_Swe1KO_UbP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Apubscrawl_Swe1KO_WCL		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Apubscrawl_Swe1KO_WCLP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Control_Ub		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Control_UbP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Control_WCL		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Control_WCLP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type EtOH_Kin3KO_Ub		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type EtOH_Kin3KO_UbP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type EtOH_Kin3KO_WCL		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type EtOH_Kin3KO_WCLP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type EtOH_menadione_Ub		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type EtOH_menadione_UbP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type EtOH_menadione_WCL		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type EtOH_menadione_WCLP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Onion_At1KO_Ub		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Onion_At1KO_UbP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Onion_At1KO_WCL		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Onion_At1KO_WCLP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Onion_rapamycin_Ub		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Onion_rapamycin_UbP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Onion_rapamycin_WCL		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Onion_rapamycin_WCLP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Pynd_5FC_Ub		Indicates whether this experiment was identified by MS/MS or only by matching between runs.

Identification type Pynd_5FC_UbP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Pynd_5FC_WCL		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Pynd_5FC_WCLP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Pynd_AlkKO_Ub		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Pynd_AlkKO_UbP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Pynd_AlkKO_WCL		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Pynd_AlkKO_WCLP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Shmoo_CaCl2_Ub		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Shmoo_CaCl2_WCL		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Shmoo_Cmk1KO_Ub		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Shmoo_Cmk1KO_UbP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Shmoo_Cmk1KO_WCL		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Shmoo_Cmk1KO_WCLP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Whangee_Tpk1KO_Ub		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Whangee_Tpk1KO_UbP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Whangee_Tpk1KO_WCL		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Whangee_Tpk1KO_WCLP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Whangee_tunicamycin_Ub		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Whangee_tunicamycin_UbP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Whangee_tunicamycin_WCL		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Whangee_tunicamycin_WCLP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
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___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___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___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.
Ratio mod/base		
Intensity Apubscrawl_Cerulenin_Ub		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 Apubscrawl_Cerulenin_UbP		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 Apubscrawl_Cerulenin_WCL		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 Apubscrawl_Cerulenin_WCLP		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 Apubscrawl_Swe1KO_Ub		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.



[illegible]

[illegible]

Intensity Whangee_tunicamycin_UbP		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 Whangee_tunicamycin_WCL		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 Whangee_tunicamycin_WCLP		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 Apubscrawl_Cerulenin_Ub		
Ratio mod/base Apubscrawl_Cerulenin_UbP		
Ratio mod/base Apubscrawl_Cerulenin_WCL		
Ratio mod/base Apubscrawl_Cerulenin_WCLP		
Ratio mod/base Apubscrawl_Swe1KO_Ub		
Ratio mod/base Apubscrawl_Swe1KO_UbP		
Ratio mod/base Apubscrawl_Swe1KO_WCL		
Ratio mod/base Apubscrawl_Swe1KO_WCLP		
Ratio mod/base Control_Ub		
Ratio mod/base Control_UbP		
Ratio mod/base Control_WCL		
Ratio mod/base Control_WCLP		
Ratio mod/base EtOH_Kin3KO_Ub		
Ratio mod/base EtOH_Kin3KO_UbP		
Ratio mod/base EtOH_Kin3KO_WCL		
Ratio mod/base EtOH_Kin3KO_WCLP		
Ratio mod/base EtOH_menadione_Ub		
Ratio mod/base EtOH_menadione_UbP		
Ratio mod/base EtOH_menadione_WCL		
Ratio mod/base EtOH_menadione_WCLP		
Ratio mod/base Onion_At1KO_Ub		
Ratio mod/base Onion_At1KO_UbP		
Ratio mod/base Onion_At1KO_WCL		
Ratio mod/base Onion_At1KO_WCLP		
Ratio mod/base Onion_rapamycin_Ub		
Ratio mod/base Onion_rapamycin_UbP		
Ratio mod/base Onion_rapamycin_WCL		
Ratio mod/base Onion_rapamycin_WCLP		
Ratio mod/base Pynd_5FC_Ub		
Ratio mod/base Pynd_5FC_UbP		
Ratio mod/base Pynd_5FC_WCL		
Ratio mod/base Pynd_5FC_WCLP		
Ratio mod/base Pynd_Al1KO_Ub		
Ratio mod/base Pynd_Al1KO_UbP		
Ratio mod/base Pynd_Al1KO_WCL		
Ratio mod/base Pynd_Al1KO_WCLP		
Ratio mod/base Shmoo_CaCl2_Ub		
Ratio mod/base Shmoo_CaCl2_WCL		

[illegible]

[illegible]

[illegible]

[illegible]

[illegible]



[illegible]

[illegible]

Intensity Whangee_tunicamycin_Ub___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 Whangee_tunicamycin_UbP___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 Whangee_tunicamycin_UbP___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 Whangee_tunicamycin_UbP___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 Whangee_tunicamycin_WCL___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 Whangee_tunicamycin_WCL___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 Whangee_tunicamycin_WCL___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 Whangee_tunicamycin_WCLP___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 Whangee_tunicamycin_WCLP___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 Whangee_tunicamycin_WCLP___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 evidences 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		

# Phospho (STY)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 Apubscrawl_Cerulenin_Ub		
Score diff Apubscrawl_Cerulenin_Ub		
PEP Apubscrawl_Cerulenin_Ub		
Score Apubscrawl_Cerulenin_Ub		
Localization prob Apubscrawl_Cerulenin_UbP		
Score diff Apubscrawl_Cerulenin_UbP		
PEP Apubscrawl_Cerulenin_UbP		
Score Apubscrawl_Cerulenin_UbP		
Localization prob Apubscrawl_Cerulenin_WCL		
Score diff Apubscrawl_Cerulenin_WCL		
PEP Apubscrawl_Cerulenin_WCL		
Score Apubscrawl_Cerulenin_WCL		
Localization prob Apubscrawl_Cerulenin_WCLP		
Score diff Apubscrawl_Cerulenin_WCLP		
PEP Apubscrawl_Cerulenin_WCLP		
Score Apubscrawl_Cerulenin_WCLP		
Localization prob Apubscrawl_Swe1KO_Ub		
Score diff Apubscrawl_Swe1KO_Ub		
PEP Apubscrawl_Swe1KO_Ub		
Score Apubscrawl_Swe1KO_Ub		
Localization prob Apubscrawl_Swe1KO_UbP		
Score diff Apubscrawl_Swe1KO_UbP		
PEP Apubscrawl_Swe1KO_UbP		
Score Apubscrawl_Swe1KO_UbP		
Localization prob Apubscrawl_Swe1KO_WCL		
Score diff Apubscrawl_Swe1KO_WCL		
PEP Apubscrawl_Swe1KO_WCL		
Score Apubscrawl_Swe1KO_WCL		
Localization prob Apubscrawl_Swe1KO_WCLP		
Score diff Apubscrawl_Swe1KO_WCLP		
PEP Apubscrawl_Swe1KO_WCLP		
Score Apubscrawl_Swe1KO_WCLP		

Localization prob Control_Ub		
Score diff Control_Ub		
PEP Control_Ub		
Score Control_Ub		
Localization prob Control_UbP		
Score diff Control_UbP		
PEP Control_UbP		
Score Control_UbP		
Localization prob Control_WCL		
Score diff Control_WCL		
PEP Control_WCL		
Score Control_WCL		
Localization prob Control_WCLP		
Score diff Control_WCLP		
PEP Control_WCLP		
Score Control_WCLP		
Localization prob EtOH_Kin3KO_Ub		
Score diff EtOH_Kin3KO_Ub		
PEP EtOH_Kin3KO_Ub		
Score EtOH_Kin3KO_Ub		
Localization prob EtOH_Kin3KO_UbP		
Score diff EtOH_Kin3KO_UbP		
PEP EtOH_Kin3KO_UbP		
Score EtOH_Kin3KO_UbP		
Localization prob EtOH_Kin3KO_WCL		
Score diff EtOH_Kin3KO_WCL		
PEP EtOH_Kin3KO_WCL		
Score EtOH_Kin3KO_WCL		
Localization prob EtOH_Kin3KO_WCLP		
Score diff EtOH_Kin3KO_WCLP		
PEP EtOH_Kin3KO_WCLP		
Score EtOH_Kin3KO_WCLP		
Localization prob EtOH_menadione_Ub		
Score diff EtOH_menadione_Ub		
PEP EtOH_menadione_Ub		
Score EtOH_menadione_Ub		
Localization prob EtOH_menadione_UbP		
Score diff EtOH_menadione_UbP		
PEP EtOH_menadione_UbP		
Score EtOH_menadione_UbP		
Localization prob EtOH_menadione_WCL		
Score diff EtOH_menadione_WCL		
PEP EtOH_menadione_WCL		
Score EtOH_menadione_WCL		
Localization prob EtOH_menadione_WCLP		
Score diff EtOH_menadione_WCLP		
PEP EtOH_menadione_WCLP		
Score EtOH_menadione_WCLP		
Localization prob Onion_Atg1KO_Ub		
Score diff Onion_Atg1KO_Ub		
PEP Onion_Atg1KO_Ub		
Score Onion_Atg1KO_Ub		
Localization prob Onion_Atg1KO_UbP		
Score diff Onion_Atg1KO_UbP		
PEP Onion_Atg1KO_UbP		
Score Onion_Atg1KO_UbP		
Localization prob Onion_Atg1KO_WCL		

Score diff Onion_Atg1KO_WCL		
PEP Onion_Atg1KO_WCL		
Score Onion_Atg1KO_WCL		
Localization prob Onion_Atg1KO_WCLP		
Score diff Onion_Atg1KO_WCLP		
PEP Onion_Atg1KO_WCLP		
Score Onion_Atg1KO_WCLP		
Localization prob Onion_rapamycin_Ub		
Score diff Onion_rapamycin_Ub		
PEP Onion_rapamycin_Ub		
Score Onion_rapamycin_Ub		
Localization prob Onion_rapamycin_UbP		
Score diff Onion_rapamycin_UbP		
PEP Onion_rapamycin_UbP		
Score Onion_rapamycin_UbP		
Localization prob Onion_rapamycin_WCL		
Score diff Onion_rapamycin_WCL		
PEP Onion_rapamycin_WCL		
Score Onion_rapamycin_WCL		
Localization prob Onion_rapamycin_WCLP		
Score diff Onion_rapamycin_WCLP		
PEP Onion_rapamycin_WCLP		
Score Onion_rapamycin_WCLP		
Localization prob Pynd_5FC_Ub		
Score diff Pynd_5FC_Ub		
PEP Pynd_5FC_Ub		
Score Pynd_5FC_Ub		
Localization prob Pynd_5FC_UbP		
Score diff Pynd_5FC_UbP		
PEP Pynd_5FC_UbP		
Score Pynd_5FC_UbP		
Localization prob Pynd_5FC_WCL		
Score diff Pynd_5FC_WCL		
PEP Pynd_5FC_WCL		
Score Pynd_5FC_WCL		
Localization prob Pynd_5FC_WCLP		
Score diff Pynd_5FC_WCLP		
PEP Pynd_5FC_WCLP		
Score Pynd_5FC_WCLP		
Localization prob Pynd_AlkKO_Ub		
Score diff Pynd_AlkKO_Ub		
PEP Pynd_AlkKO_Ub		
Score Pynd_AlkKO_Ub		
Localization prob Pynd_AlkKO_UbP		
Score diff Pynd_AlkKO_UbP		
PEP Pynd_AlkKO_UbP		
Score Pynd_AlkKO_UbP		
Localization prob Pynd_AlkKO_WCL		
Score diff Pynd_AlkKO_WCL		
PEP Pynd_AlkKO_WCL		
Score Pynd_AlkKO_WCL		
Localization prob Pynd_AlkKO_WCLP		
Score diff Pynd_AlkKO_WCLP		
PEP Pynd_AlkKO_WCLP		
Score Pynd_AlkKO_WCLP		
Localization prob Shmoo_CaCl2_Ub		
Score diff Shmoo_CaCl2_Ub		
PEP Shmoo_CaCl2_Ub		

Score Shmoo_CaCl2_Ub		
Localization prob Shmoo_CaCl2_WCL		
Score diff Shmoo_CaCl2_WCL		
PEP Shmoo_CaCl2_WCL		
Score Shmoo_CaCl2_WCL		
Localization prob Shmoo_Cmk1KO_Ub		
Score diff Shmoo_Cmk1KO_Ub		
PEP Shmoo_Cmk1KO_Ub		
Score Shmoo_Cmk1KO_Ub		
Localization prob Shmoo_Cmk1KO_UbP		
Score diff Shmoo_Cmk1KO_UbP		
PEP Shmoo_Cmk1KO_UbP		
Score Shmoo_Cmk1KO_UbP		
Localization prob Shmoo_Cmk1KO_WCL		
Score diff Shmoo_Cmk1KO_WCL		
PEP Shmoo_Cmk1KO_WCL		
Score Shmoo_Cmk1KO_WCL		
Localization prob Shmoo_Cmk1KO_WCLP		
Score diff Shmoo_Cmk1KO_WCLP		
PEP Shmoo_Cmk1KO_WCLP		
Score Shmoo_Cmk1KO_WCLP		
Localization prob Whangee_Tpk1KO_Ub		
Score diff Whangee_Tpk1KO_Ub		
PEP Whangee_Tpk1KO_Ub		
Score Whangee_Tpk1KO_Ub		
Localization prob Whangee_Tpk1KO_UbP		
Score diff Whangee_Tpk1KO_UbP		
PEP Whangee_Tpk1KO_UbP		
Score Whangee_Tpk1KO_UbP		
Localization prob Whangee_Tpk1KO_WCL		
Score diff Whangee_Tpk1KO_WCL		
PEP Whangee_Tpk1KO_WCL		
Score Whangee_Tpk1KO_WCL		
Localization prob Whangee_Tpk1KO_WCLP		
Score diff Whangee_Tpk1KO_WCLP		
PEP Whangee_Tpk1KO_WCLP		
Score Whangee_Tpk1KO_WCLP		
Localization prob Whangee_tunicamycin_Ub		
Score diff Whangee_tunicamycin_Ub		
PEP Whangee_tunicamycin_Ub		
Score Whangee_tunicamycin_Ub		
Localization prob Whangee_tunicamycin_UbP		
Score diff Whangee_tunicamycin_UbP		
PEP Whangee_tunicamycin_UbP		
Score Whangee_tunicamycin_UbP		
Localization prob Whangee_tunicamycin_WCL		
Score diff Whangee_tunicamycin_WCL		
PEP Whangee_tunicamycin_WCL		
Score Whangee_tunicamycin_WCL		
Localization prob Whangee_tunicamycin_WCLP		
Score diff Whangee_tunicamycin_WCLP		
PEP Whangee_tunicamycin_WCLP		



Score		
Whangee_tunicamycin_WCLP		
Diagnostic peak		
Number of Phospho (STY)		Different numbers of Phospho (STY) on peptides that this site is involved in.
Amino acid		
Sequence window		
Modification window		
Peptide window coverage		
Phospho (STY) Probabilities		
Phospho (STY) 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		
Apubscrawl_Cerulenin_Ub		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type		
Apubscrawl_Cerulenin_UbP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type		
Apubscrawl_Cerulenin_WCL		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type		
Apubscrawl_Cerulenin_WCLP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type		
Apubscrawl_Swe1KO_Ub		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type		
Apubscrawl_Swe1KO_UbP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type		
Apubscrawl_Swe1KO_WCL		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type		
Apubscrawl_Swe1KO_WCLP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Control_Ub		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Control_UbP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Control_WCL		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Control_WCLP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type		
EtOH_Kin3KO_Ub		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type		
EtOH_Kin3KO_UbP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type		
EtOH_Kin3KO_WCL		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type		
EtOH_Kin3KO_WCLP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type		
EtOH_menadione_Ub		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type		
EtOH_menadione_UbP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type		
EtOH_menadione_WCL		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type		
EtOH_menadione_WCLP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type		
Onion_At1KO_Ub		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type		
Onion_At1KO_UbP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type		
Onion_At1KO_WCL		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type		
Onion_At1KO_WCLP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type		
Onion_rapamycin_Ub		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type		
Onion_rapamycin_UbP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type		
Onion_rapamycin_WCL		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type		
Onion_rapamycin_WCLP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Pynd_5FC_Ub		Indicates whether this experiment was identified by MS/MS or only by matching between runs.

Identification type Pynd_5FC_UbP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Pynd_5FC_WCL		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Pynd_5FC_WCLP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Pynd_AlkKO_Ub		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Pynd_AlkKO_UbP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Pynd_AlkKO_WCL		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Pynd_AlkKO_WCLP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Shmoo_CaCl2_Ub		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Shmoo_CaCl2_WCL		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Shmoo_Cmk1KO_Ub		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Shmoo_Cmk1KO_UbP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Shmoo_Cmk1KO_WCL		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Shmoo_Cmk1KO_WCLP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Whangee_Tpk1KO_Ub		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Whangee_Tpk1KO_UbP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Whangee_Tpk1KO_WCL		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Whangee_Tpk1KO_WCLP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Whangee_tunicamycin_Ub		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Whangee_tunicamycin_UbP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Whangee_tunicamycin_WCL		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Whangee_tunicamycin_WCLP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
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___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___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___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.
Ratio mod/base		
Intensity Apubscrawl_Cerulenin_Ub		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 Apubscrawl_Cerulenin_UbP		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 Apubscrawl_Cerulenin_WCL		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 Apubscrawl_Cerulenin_WCLP		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 Apubscrawl_Swe1KO_Ub		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.

[illegible]

[illegible]

Intensity Whangee_tunicamycin_UbP		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 Whangee_tunicamycin_WCL		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 Whangee_tunicamycin_WCLP		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 Apubscrawl_Cerulenin_Ub		
Ratio mod/base Apubscrawl_Cerulenin_UbP		
Ratio mod/base Apubscrawl_Cerulenin_WCL		
Ratio mod/base Apubscrawl_Cerulenin_WCLP		
Ratio mod/base Apubscrawl_Swe1KO_Ub		
Ratio mod/base Apubscrawl_Swe1KO_UbP		
Ratio mod/base Apubscrawl_Swe1KO_WCL		
Ratio mod/base Apubscrawl_Swe1KO_WCLP		
Ratio mod/base Control_Ub		
Ratio mod/base Control_UbP		
Ratio mod/base Control_WCL		
Ratio mod/base Control_WCLP		
Ratio mod/base EtOH_Kin3KO_Ub		
Ratio mod/base EtOH_Kin3KO_UbP		
Ratio mod/base EtOH_Kin3KO_WCL		
Ratio mod/base EtOH_Kin3KO_WCLP		
Ratio mod/base EtOH_menadione_Ub		
Ratio mod/base EtOH_menadione_UbP		
Ratio mod/base EtOH_menadione_WCL		
Ratio mod/base EtOH_menadione_WCLP		
Ratio mod/base Onion_At1KO_Ub		
Ratio mod/base Onion_At1KO_UbP		
Ratio mod/base Onion_At1KO_WCL		
Ratio mod/base Onion_At1KO_WCLP		
Ratio mod/base Onion_rapamycin_Ub		
Ratio mod/base Onion_rapamycin_UbP		
Ratio mod/base Onion_rapamycin_WCL		
Ratio mod/base Onion_rapamycin_WCLP		
Ratio mod/base Pynd_5FC_Ub		
Ratio mod/base Pynd_5FC_UbP		
Ratio mod/base Pynd_5FC_WCL		
Ratio mod/base Pynd_5FC_WCLP		
Ratio mod/base Pynd_Al1KO_Ub		
Ratio mod/base Pynd_Al1KO_UbP		
Ratio mod/base Pynd_Al1KO_WCL		
Ratio mod/base Pynd_Al1KO_WCLP		
Ratio mod/base Shmoo_CaCl2_Ub		
Ratio mod/base Shmoo_CaCl2_WCL		

[illegible]

[illegible]

[illegible]



[illegible]

[illegible]

[illegible]

[illegible]

Intensity Whangee_tunicamycin_Ub___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 Whangee_tunicamycin_UbP___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 Whangee_tunicamycin_UbP___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 Whangee_tunicamycin_UbP___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 Whangee_tunicamycin_WCL___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 Whangee_tunicamycin_WCL___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 Whangee_tunicamycin_WCL___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 Whangee_tunicamycin_WCLP___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 Whangee_tunicamycin_WCLP___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 Whangee_tunicamycin_WCLP___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 Apubscrawl_Cerulenin_Ub		
Occupancy ratioApubscrawl_Cerulenin_Ub		
Occupancy error scale Apubscrawl_Cerulenin_Ub		
Occupancy Apubscrawl_Cerulenin_UbP		
Occupancy ratioApubscrawl_Cerulenin_UbP		
Occupancy error scale Apubscrawl_Cerulenin_UbP		
Occupancy Apubscrawl_Cerulenin_WCL		
Occupancy ratioApubscrawl_Cerulenin_WCL		
Occupancy error scale Apubscrawl_Cerulenin_WCL		
Occupancy Apubscrawl_Cerulenin_WCLP		
Occupancy ratioApubscrawl_Cerulenin_WCLP		
Occupancy error scale Apubscrawl_Cerulenin_WCLP		
Occupancy Apubscrawl_Swe1KO_Ub		
Occupancy ratioApubscrawl_Swe1KO_Ub		
Occupancy error scale Apubscrawl_Swe1KO_Ub		
Occupancy Apubscrawl_Swe1KO_UbP		
Occupancy ratioApubscrawl_Swe1KO_UbP		
Occupancy error scale Apubscrawl_Swe1KO_UbP		
Occupancy Apubscrawl_Swe1KO_WCL		
Occupancy ratioApubscrawl_Swe1KO_WCL		

Occupancy error scale Apubscrawl_Swe1KO_WCL		
Occupancy Apubscrawl_Swe1KO_WCLP		
Occupancy ratioApubscrawl_Swe1KO_WCLP		
Occupancy error scale Apubscrawl_Swe1KO_WCLP		
Occupancy Control_Ub		
Occupancy ratioControl_Ub		
Occupancy error scale Control_Ub		
Occupancy Control_UbP		
Occupancy ratioControl_UbP		
Occupancy error scale Control_UbP		
Occupancy Control_WCL		
Occupancy ratioControl_WCL		
Occupancy error scale Control_WCL		
Occupancy Control_WCLP		
Occupancy ratioControl_WCLP		
Occupancy error scale Control_WCLP		
Occupancy EtOH_Kin3KO_Ub		
Occupancy ratioEtOH_Kin3KO_Ub		
Occupancy error scale EtOH_Kin3KO_Ub		
Occupancy EtOH_Kin3KO_UbP		
Occupancy ratioEtOH_Kin3KO_UbP		
Occupancy error scale EtOH_Kin3KO_UbP		
Occupancy EtOH_Kin3KO_WCL		
Occupancy ratioEtOH_Kin3KO_WCL		
Occupancy error scale EtOH_Kin3KO_WCL		
Occupancy EtOH_Kin3KO_WCLP		
Occupancy ratioEtOH_Kin3KO_WCLP		
Occupancy error scale EtOH_Kin3KO_WCLP		
Occupancy EtOH_menadione_Ub		
Occupancy ratioEtOH_menadione_Ub		
Occupancy error scale EtOH_menadione_Ub		
Occupancy EtOH_menadione_UbP		
Occupancy ratioEtOH_menadione_UbP		
Occupancy error scale EtOH_menadione_UbP		
Occupancy EtOH_menadione_WCL		
Occupancy ratioEtOH_menadione_WCL		
Occupancy error scale EtOH_menadione_WCL		
Occupancy EtOH_menadione_WCLP		
Occupancy ratioEtOH_menadione_WCLP		
Occupancy error scale EtOH_menadione_WCLP		
Occupancy Onion_Atq1KO_Ub		
Occupancy ratioOnion_Atq1KO_Ub		
Occupancy error scale Onion_Atq1KO_Ub		
Occupancy Onion_Atq1KO_UbP		
Occupancy ratioOnion_Atq1KO_UbP		
Occupancy error scale Onion_Atq1KO_UbP		
Occupancy Onion_Atq1KO_WCL		

Occupancy ratioOnion_At91KO_WCL		
Occupancy error scale Onion_At91KO_WCL		
Occupancy Onion_At91KO_WCLP		
Occupancy ratioOnion_At91KO_WCLP		
Occupancy error scale Onion_At91KO_WCLP		
Occupancy Onion_rapamycin_Ub		
Occupancy ratioOnion_rapamycin_Ub		
Occupancy error scale Onion_rapamycin_Ub		
Occupancy Onion_rapamycin_UbP		
Occupancy ratioOnion_rapamycin_UbP		
Occupancy error scale Onion_rapamycin_UbP		
Occupancy Onion_rapamycin_WCL		
Occupancy ratioOnion_rapamycin_WCL		
Occupancy error scale Onion_rapamycin_WCL		
Occupancy Onion_rapamycin_WCLP		
Occupancy ratioOnion_rapamycin_WCLP		
Occupancy error scale Onion_rapamycin_WCLP		
Occupancy Pynd_5FC_Ub		
Occupancy ratioPynd_5FC_Ub		
Occupancy error scale Pynd_5FC_Ub		
Occupancy Pynd_5FC_UbP		
Occupancy ratioPynd_5FC_UbP		
Occupancy error scale Pynd_5FC_UbP		
Occupancy Pynd_5FC_WCL		
Occupancy ratioPynd_5FC_WCL		
Occupancy error scale Pynd_5FC_WCL		
Occupancy Pynd_5FC_WCLP		
Occupancy ratioPynd_5FC_WCLP		
Occupancy error scale Pynd_5FC_WCLP		
Occupancy Pynd_AlkKO_Ub		
Occupancy ratioPynd_AlkKO_Ub		
Occupancy error scale Pynd_AlkKO_Ub		
Occupancy Pynd_AlkKO_UbP		
Occupancy ratioPynd_AlkKO_UbP		
Occupancy error scale Pynd_AlkKO_UbP		
Occupancy Pynd_AlkKO_WCL		
Occupancy ratioPynd_AlkKO_WCL		
Occupancy error scale Pynd_AlkKO_WCL		
Occupancy Pynd_AlkKO_WCLP		
Occupancy ratioPynd_AlkKO_WCLP		
Occupancy error scale Pynd_AlkKO_WCLP		
Occupancy Shmoo_CaCl2_Ub		
Occupancy ratioShmoo_CaCl2_Ub		
Occupancy error scale Shmoo_CaCl2_Ub		
Occupancy Shmoo_CaCl2_WCL		
Occupancy ratioShmoo_CaCl2_WCL		
Occupancy error scale Shmoo_CaCl2_WCL		

Occupancy Shmoo_Cmk1KO_Ub		
Occupancy ratioShmoo_Cmk1KO_Ub		
Occupancy error scale Shmoo_Cmk1KO_Ub		
Occupancy Shmoo_Cmk1KO_UbP		
Occupancy ratioShmoo_Cmk1KO_UbP		
Occupancy error scale Shmoo_Cmk1KO_UbP		
Occupancy Shmoo_Cmk1KO_WCL		
Occupancy ratioShmoo_Cmk1KO_WCL		
Occupancy error scale Shmoo_Cmk1KO_WCL		
Occupancy Shmoo_Cmk1KO_WCLP		
Occupancy ratioShmoo_Cmk1KO_WCLP		
Occupancy error scale Shmoo_Cmk1KO_WCLP		
Occupancy Whangee_Tpk1KO_Ub		
Occupancy ratioWhangee_Tpk1KO_Ub		
Occupancy error scale Whangee_Tpk1KO_Ub		
Occupancy Whangee_Tpk1KO_UbP		
Occupancy ratioWhangee_Tpk1KO_UbP		
Occupancy error scale Whangee_Tpk1KO_UbP		
Occupancy Whangee_Tpk1KO_WCL		
Occupancy ratioWhangee_Tpk1KO_WCL		
Occupancy error scale Whangee_Tpk1KO_WCL		
Occupancy Whangee_Tpk1KO_WCLP		
Occupancy ratioWhangee_Tpk1KO_WCLP		
Occupancy error scale Whangee_Tpk1KO_WCLP		
Occupancy Whangee_tunicamycin_Ub		
Occupancy ratioWhangee_tunicamycin_Ub		
Occupancy error scale Whangee_tunicamycin_Ub		
Occupancy Whangee_tunicamycin_UbP		
Occupancy ratioWhangee_tunicamycin_UbP		
Occupancy error scale Whangee_tunicamycin_UbP		
Occupancy Whangee_tunicamycin_WCL		
Occupancy ratioWhangee_tunicamycin_WCL		
Occupancy error scale Whangee_tunicamycin_WCL		
Occupancy Whangee_tunicamycin_WCLP		
Occupancy ratioWhangee_tunicamycin_WCLP		
Occupancy error scale Whangee_tunicamycin_WCLP		
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 evidences 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		Identifier(s) of protein(s) 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 Apubscrawl_Cerulenin_Ub		Number of peptides (distinct peptide sequences) in experiment Apubscrawl_Cerulenin_Ub
Peptides Apubscrawl_Cerulenin_UbP		Number of peptides (distinct peptide sequences) in experiment Apubscrawl_Cerulenin_UbP
Peptides Apubscrawl_Cerulenin_WCL		Number of peptides (distinct peptide sequences) in experiment Apubscrawl_Cerulenin_WCL
Peptides Apubscrawl_Cerulenin_WCLP		Number of peptides (distinct peptide sequences) in experiment Apubscrawl_Cerulenin_WCLP
Peptides Apubscrawl_Swe1KO_Ub		Number of peptides (distinct peptide sequences) in experiment Apubscrawl_Swe1KO_Ub
Peptides Apubscrawl_Swe1KO_UbP		Number of peptides (distinct peptide sequences) in experiment Apubscrawl_Swe1KO_UbP
Peptides Apubscrawl_Swe1KO_WCL		Number of peptides (distinct peptide sequences) in experiment Apubscrawl_Swe1KO_WCL
Peptides Apubscrawl_Swe1KO_WCLP		Number of peptides (distinct peptide sequences) in experiment Apubscrawl_Swe1KO_WCLP
Peptides Control_Ub		Number of peptides (distinct peptide sequences) in experiment Control_Ub
Peptides Control_UbP		Number of peptides (distinct peptide sequences) in experiment Control_UbP
Peptides Control_WCL		Number of peptides (distinct peptide sequences) in experiment Control_WCL
Peptides Control_WCLP		Number of peptides (distinct peptide sequences) in experiment Control_WCLP
Peptides EtOH_Kin3KO_Ub		Number of peptides (distinct peptide sequences) in experiment EtOH_Kin3KO_Ub
Peptides EtOH_Kin3KO_UbP		Number of peptides (distinct peptide sequences) in experiment EtOH_Kin3KO_UbP
Peptides EtOH_Kin3KO_WCL		Number of peptides (distinct peptide sequences) in experiment EtOH_Kin3KO_WCL
Peptides EtOH_Kin3KO_WCLP		Number of peptides (distinct peptide sequences) in experiment EtOH_Kin3KO_WCLP
Peptides EtOH_menadione_Ub		Number of peptides (distinct peptide sequences) in experiment EtOH_menadione_Ub
Peptides EtOH_menadione_UbP		Number of peptides (distinct peptide sequences) in experiment EtOH_menadione_UbP

Peptides EtOH_menadione_WCL		Number of peptides (distinct peptide sequences) in experiment EtOH_menadione_WCL
Peptides EtOH_menadione_WCLP		Number of peptides (distinct peptide sequences) in experiment EtOH_menadione_WCLP
Peptides Onion_Atg1KO_Ub		Number of peptides (distinct peptide sequences) in experiment Onion_Atg1KO_Ub
Peptides Onion_Atg1KO_UbP		Number of peptides (distinct peptide sequences) in experiment Onion_Atg1KO_UbP
Peptides Onion_Atg1KO_WCL		Number of peptides (distinct peptide sequences) in experiment Onion_Atg1KO_WCL
Peptides Onion_Atg1KO_WCLP		Number of peptides (distinct peptide sequences) in experiment Onion_Atg1KO_WCLP
Peptides Onion_rapamycin_Ub		Number of peptides (distinct peptide sequences) in experiment Onion_rapamycin_Ub
Peptides Onion_rapamycin_UbP		Number of peptides (distinct peptide sequences) in experiment Onion_rapamycin_UbP
Peptides Onion_rapamycin_WCL		Number of peptides (distinct peptide sequences) in experiment Onion_rapamycin_WCL
Peptides Onion_rapamycin_WCLP		Number of peptides (distinct peptide sequences) in experiment Onion_rapamycin_WCLP
Peptides Pynd_5FC_Ub		Number of peptides (distinct peptide sequences) in experiment Pynd_5FC_Ub
Peptides Pynd_5FC_UbP		Number of peptides (distinct peptide sequences) in experiment Pynd_5FC_UbP
Peptides Pynd_5FC_WCL		Number of peptides (distinct peptide sequences) in experiment Pynd_5FC_WCL
Peptides Pynd_5FC_WCLP		Number of peptides (distinct peptide sequences) in experiment Pynd_5FC_WCLP
Peptides Pynd_AlkkO_Ub		Number of peptides (distinct peptide sequences) in experiment Pynd_AlkkO_Ub
Peptides Pynd_AlkkO_UbP		Number of peptides (distinct peptide sequences) in experiment Pynd_AlkkO_UbP
Peptides Pynd_AlkkO_WCL		Number of peptides (distinct peptide sequences) in experiment Pynd_AlkkO_WCL
Peptides Pynd_AlkkO_WCLP		Number of peptides (distinct peptide sequences) in experiment Pynd_AlkkO_WCLP
Peptides Shmoo_CaCl2_Ub		Number of peptides (distinct peptide sequences) in experiment Shmoo_CaCl2_Ub
Peptides Shmoo_CaCl2_WCL		Number of peptides (distinct peptide sequences) in experiment Shmoo_CaCl2_WCL
Peptides Shmoo_Cmk1KO_Ub		Number of peptides (distinct peptide sequences) in experiment Shmoo_Cmk1KO_Ub
Peptides Shmoo_Cmk1KO_UbP		Number of peptides (distinct peptide sequences) in experiment Shmoo_Cmk1KO_UbP
Peptides Shmoo_Cmk1KO_WCL		Number of peptides (distinct peptide sequences) in experiment Shmoo_Cmk1KO_WCL
Peptides Shmoo_Cmk1KO_WCLP		Number of peptides (distinct peptide sequences) in experiment Shmoo_Cmk1KO_WCLP
Peptides Whangee_Tpk1KO_Ub		Number of peptides (distinct peptide sequences) in experiment Whangee_Tpk1KO_Ub
Peptides Whangee_Tpk1KO_UbP		Number of peptides (distinct peptide sequences) in experiment Whangee_Tpk1KO_UbP
Peptides Whangee_Tpk1KO_WCL		Number of peptides (distinct peptide sequences) in experiment Whangee_Tpk1KO_WCL
Peptides Whangee_Tpk1KO_WCLP		Number of peptides (distinct peptide sequences) in experiment Whangee_Tpk1KO_WCLP
Peptides Whangee_tunicamycin_Ub		Number of peptides (distinct peptide sequences) in experiment Whangee_tunicamycin_Ub
Peptides Whangee_tunicamycin_UbP		Number of peptides (distinct peptide sequences) in experiment Whangee_tunicamycin_UbP
Peptides Whangee_tunicamycin_WCL		Number of peptides (distinct peptide sequences) in experiment Whangee_tunicamycin_WCL
Peptides Whangee_tunicamycin_WCLP		Number of peptides (distinct peptide sequences) in experiment Whangee_tunicamycin_WCLP
Razor + unique peptides Apubscrawl_Cerulenin_Ub		Number of razor + unique peptides (distinct peptide sequences) in experiment Apubscrawl_Cerulenin_Ub
Razor + unique peptides Apubscrawl_Cerulenin_UbP		Number of razor + unique peptides (distinct peptide sequences) in experiment Apubscrawl_Cerulenin_UbP
Razor + unique peptides Apubscrawl_Cerulenin_WCL		Number of razor + unique peptides (distinct peptide sequences) in experiment Apubscrawl_Cerulenin_WCL
Razor + unique peptides Apubscrawl_Cerulenin_WCLP		Number of razor + unique peptides (distinct peptide sequences) in experiment Apubscrawl_Cerulenin_WCLP
Razor + unique peptides Apubscrawl_Swe1KO_Ub		Number of razor + unique peptides (distinct peptide sequences) in experiment Apubscrawl_Swe1KO_Ub
Razor + unique peptides Apubscrawl_Swe1KO_UbP		Number of razor + unique peptides (distinct peptide sequences) in experiment Apubscrawl_Swe1KO_UbP

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Razor + unique peptides Whangee_Tpk1KO_WCL		Number of razor + unique peptides (distinct peptide sequences) in experiment Whangee_Tpk1KO_WCL
Razor + unique peptides Whangee_Tpk1KO_WCLP		Number of razor + unique peptides (distinct peptide sequences) in experiment Whangee_Tpk1KO_WCLP
Razor + unique peptides Whangee_tunicamycin_Ub		Number of razor + unique peptides (distinct peptide sequences) in experiment Whangee_tunicamycin_Ub
Razor + unique peptides Whangee_tunicamycin_UbP		Number of razor + unique peptides (distinct peptide sequences) in experiment Whangee_tunicamycin_UbP
Razor + unique peptides Whangee_tunicamycin_WCL		Number of razor + unique peptides (distinct peptide sequences) in experiment Whangee_tunicamycin_WCL
Razor + unique peptides Whangee_tunicamycin_WCLP		Number of razor + unique peptides (distinct peptide sequences) in experiment Whangee_tunicamycin_WCLP
Unique peptides Apubscrawl_Cerulenin_Ub		Number of unique peptides (distinct peptide sequences) in experiment Apubscrawl_Cerulenin_Ub
Unique peptides Apubscrawl_Cerulenin_UbP		Number of unique peptides (distinct peptide sequences) in experiment Apubscrawl_Cerulenin_UbP
Unique peptides Apubscrawl_Cerulenin_WCL		Number of unique peptides (distinct peptide sequences) in experiment Apubscrawl_Cerulenin_WCL
Unique peptides Apubscrawl_Cerulenin_WCLP		Number of unique peptides (distinct peptide sequences) in experiment Apubscrawl_Cerulenin_WCLP
Unique peptides Apubscrawl_Swe1KO_Ub		Number of unique peptides (distinct peptide sequences) in experiment Apubscrawl_Swe1KO_Ub
Unique peptides Apubscrawl_Swe1KO_UbP		Number of unique peptides (distinct peptide sequences) in experiment Apubscrawl_Swe1KO_UbP
Unique peptides Apubscrawl_Swe1KO_WCL		Number of unique peptides (distinct peptide sequences) in experiment Apubscrawl_Swe1KO_WCL
Unique peptides Apubscrawl_Swe1KO_WCLP		Number of unique peptides (distinct peptide sequences) in experiment Apubscrawl_Swe1KO_WCLP
Unique peptides Control_Ub		Number of unique peptides (distinct peptide sequences) in experiment Control_Ub
Unique peptides Control_UbP		Number of unique peptides (distinct peptide sequences) in experiment Control_UbP
Unique peptides Control_WCL		Number of unique peptides (distinct peptide sequences) in experiment Control_WCL
Unique peptides Control_WCLP		Number of unique peptides (distinct peptide sequences) in experiment Control_WCLP
Unique peptides EtOH_Kin3KO_Ub		Number of unique peptides (distinct peptide sequences) in experiment EtOH_Kin3KO_Ub
Unique peptides EtOH_Kin3KO_UbP		Number of unique peptides (distinct peptide sequences) in experiment EtOH_Kin3KO_UbP
Unique peptides EtOH_Kin3KO_WCL		Number of unique peptides (distinct peptide sequences) in experiment EtOH_Kin3KO_WCL
Unique peptides EtOH_Kin3KO_WCLP		Number of unique peptides (distinct peptide sequences) in experiment EtOH_Kin3KO_WCLP
Unique peptides EtOH_menadione_Ub		Number of unique peptides (distinct peptide sequences) in experiment EtOH_menadione_Ub
Unique peptides EtOH_menadione_UbP		Number of unique peptides (distinct peptide sequences) in experiment EtOH_menadione_UbP
Unique peptides EtOH_menadione_WCL		Number of unique peptides (distinct peptide sequences) in experiment EtOH_menadione_WCL
Unique peptides EtOH_menadione_WCLP		Number of unique peptides (distinct peptide sequences) in experiment EtOH_menadione_WCLP
Unique peptides Onion_Atg1KO_Ub		Number of unique peptides (distinct peptide sequences) in experiment Onion_Atg1KO_Ub
Unique peptides Onion_Atg1KO_UbP		Number of unique peptides (distinct peptide sequences) in experiment Onion_Atg1KO_UbP
Unique peptides Onion_Atg1KO_WCL		Number of unique peptides (distinct peptide sequences) in experiment Onion_Atg1KO_WCL
Unique peptides Onion_Atg1KO_WCLP		Number of unique peptides (distinct peptide sequences) in experiment Onion_Atg1KO_WCLP
Unique peptides Onion_rapamycin_Ub		Number of unique peptides (distinct peptide sequences) in experiment Onion_rapamycin_Ub
Unique peptides Onion_rapamycin_UbP		Number of unique peptides (distinct peptide sequences) in experiment Onion_rapamycin_UbP
Unique peptides Onion_rapamycin_WCL		Number of unique peptides (distinct peptide sequences) in experiment Onion_rapamycin_WCL
Unique peptides Onion_rapamycin_WCLP		Number of unique peptides (distinct peptide sequences) in experiment Onion_rapamycin_WCLP
Unique peptides Pynd_5FC_Ub		Number of unique peptides (distinct peptide sequences) in experiment Pynd_5FC_Ub
Unique peptides Pynd_5FC_UbP		Number of unique peptides (distinct peptide sequences) in experiment Pynd_5FC_UbP
Unique peptides Pynd_5FC_WCL		Number of unique peptides (distinct peptide sequences) in experiment Pynd_5FC_WCL
Unique peptides Pynd_5FC_WCLP		Number of unique peptides (distinct peptide sequences) in experiment Pynd_5FC_WCLP

Unique peptides Pynd_AlkkO_Ub		Number of unique peptides (distinct peptide sequences) in experiment Pynd_AlkkO_Ub
Unique peptides Pynd_AlkkO_UbP		Number of unique peptides (distinct peptide sequences) in experiment Pynd_AlkkO_UbP
Unique peptides Pynd_AlkkO_WCL		Number of unique peptides (distinct peptide sequences) in experiment Pynd_AlkkO_WCL
Unique peptides Pynd_AlkkO_WCLP		Number of unique peptides (distinct peptide sequences) in experiment Pynd_AlkkO_WCLP
Unique peptides Shmoo_CaCl2_Ub		Number of unique peptides (distinct peptide sequences) in experiment Shmoo_CaCl2_Ub
Unique peptides Shmoo_CaCl2_WCL		Number of unique peptides (distinct peptide sequences) in experiment Shmoo_CaCl2_WCL
Unique peptides Shmoo_Cmk1KO_Ub		Number of unique peptides (distinct peptide sequences) in experiment Shmoo_Cmk1KO_Ub
Unique peptides Shmoo_Cmk1KO_UbP		Number of unique peptides (distinct peptide sequences) in experiment Shmoo_Cmk1KO_UbP
Unique peptides Shmoo_Cmk1KO_WCL		Number of unique peptides (distinct peptide sequences) in experiment Shmoo_Cmk1KO_WCL
Unique peptides Shmoo_Cmk1KO_WCLP		Number of unique peptides (distinct peptide sequences) in experiment Shmoo_Cmk1KO_WCLP
Unique peptides Whangee_Tpk1KO_Ub		Number of unique peptides (distinct peptide sequences) in experiment Whangee_Tpk1KO_Ub
Unique peptides Whangee_Tpk1KO_UbP		Number of unique peptides (distinct peptide sequences) in experiment Whangee_Tpk1KO_UbP
Unique peptides Whangee_Tpk1KO_WCL		Number of unique peptides (distinct peptide sequences) in experiment Whangee_Tpk1KO_WCL
Unique peptides Whangee_Tpk1KO_WCLP		Number of unique peptides (distinct peptide sequences) in experiment Whangee_Tpk1KO_WCLP
Unique peptides Whangee_tunicamycin_Ub		Number of unique peptides (distinct peptide sequences) in experiment Whangee_tunicamycin_Ub
Unique peptides Whangee_tunicamycin_UbP		Number of unique peptides (distinct peptide sequences) in experiment Whangee_tunicamycin_UbP
Unique peptides Whangee_tunicamycin_WCL		Number of unique peptides (distinct peptide sequences) in experiment Whangee_tunicamycin_WCL
Unique peptides Whangee_tunicamycin_WCLP		Number of unique peptides (distinct peptide sequences) in experiment Whangee_tunicamycin_WCLP
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 Apubscrawl_Cerulenin_Ub		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Apubscrawl_Cerulenin_UbP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Apubscrawl_Cerulenin_WCL		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Apubscrawl_Cerulenin_WCLP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Apubscrawl_Swe1KO_Ub		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Apubscrawl_Swe1KO_UbP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Apubscrawl_Swe1KO_WCL		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Apubscrawl_Swe1KO_WCLP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Control_Ub		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Control_UbP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Control_WCL		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type Control_WCLP		Indicates whether this experiment was identified by MS/MS or only by matching between runs.

[illegible]

[illegible]



Sequence coverage Onion_rapamycin_WCLP [%]		Percentage of the sequence that is covered by the identified peptides in this sample of the longest protein sequence contained within the group.
Sequence coverage Pynd_5FC_Ub [%]		Percentage of the sequence that is covered by the identified peptides in this sample of the longest protein sequence contained within the group.
Sequence coverage Pynd_5FC_UbP [%]		Percentage of the sequence that is covered by the identified peptides in this sample of the longest protein sequence contained within the group.
Sequence coverage Pynd_5FC_WCL [%]		Percentage of the sequence that is covered by the identified peptides in this sample of the longest protein sequence contained within the group.
Sequence coverage Pynd_5FC_WCLP [%]		Percentage of the sequence that is covered by the identified peptides in this sample of the longest protein sequence contained within the group.
Sequence coverage Pynd_AlkkO_Ub [%]		Percentage of the sequence that is covered by the identified peptides in this sample of the longest protein sequence contained within the group.
Sequence coverage Pynd_AlkkO_UbP [%]		Percentage of the sequence that is covered by the identified peptides in this sample of the longest protein sequence contained within the group.
Sequence coverage Pynd_AlkkO_WCL [%]		Percentage of the sequence that is covered by the identified peptides in this sample of the longest protein sequence contained within the group.
Sequence coverage Pynd_AlkkO_WCLP [%]		Percentage of the sequence that is covered by the identified peptides in this sample of the longest protein sequence contained within the group.
Sequence coverage Shmoo_CaCl <sub>2</sub> _Ub [%]		Percentage of the sequence that is covered by the identified peptides in this sample of the longest protein sequence contained within the group.
Sequence coverage Shmoo_CaCl <sub>2</sub> _WCL [%]		Percentage of the sequence that is covered by the identified peptides in this sample of the longest protein sequence contained within the group.
Sequence coverage Shmoo_Cmk1KO_Ub [%]		Percentage of the sequence that is covered by the identified peptides in this sample of the longest protein sequence contained within the group.
Sequence coverage Shmoo_Cmk1KO_UbP [%]		Percentage of the sequence that is covered by the identified peptides in this sample of the longest protein sequence contained within the group.
Sequence coverage Shmoo_Cmk1KO_WCL [%]		Percentage of the sequence that is covered by the identified peptides in this sample of the longest protein sequence contained within the group.
Sequence coverage Shmoo_Cmk1KO_WCLP [%]		Percentage of the sequence that is covered by the identified peptides in this sample of the longest protein sequence contained within the group.
Sequence coverage Whangee_Tpk1KO_Ub [%]		Percentage of the sequence that is covered by the identified peptides in this sample of the longest protein sequence contained within the group.
Sequence coverage Whangee_Tpk1KO_UbP [%]		Percentage of the sequence that is covered by the identified peptides in this sample of the longest protein sequence contained within the group.
Sequence coverage Whangee_Tpk1KO_WCL [%]		Percentage of the sequence that is covered by the identified peptides in this sample of the longest protein sequence contained within the group.
Sequence coverage Whangee_Tpk1KO_WCLP [%]		Percentage of the sequence that is covered by the identified peptides in this sample of the longest protein sequence contained within the group.
Sequence coverage Whangee_tunicamycin_Ub [%]		Percentage of the sequence that is covered by the identified peptides in this sample of the longest protein sequence contained within the group.
Sequence coverage Whangee_tunicamycin_UbP [%]		Percentage of the sequence that is covered by the identified peptides in this sample of the longest protein sequence contained within the group.
Sequence coverage Whangee_tunicamycin_WCL [%]		Percentage of the sequence that is covered by the identified peptides in this sample of the longest protein sequence contained within the group.
Sequence coverage Whangee_tunicamycin_WCLP [%]		Percentage of the sequence that is covered by the identified peptides in this sample of the longest protein sequence contained within the group.
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 Apubscrawl_Cerulenin_Ub		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 Apubscrawl_Cerulenin_UbP		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.

[illegible]

[illegible]

Intensity Whangee_Tpk1KO_WCL		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 Whangee_Tpk1KO_WCLP		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 Whangee_tunicamycin_Ub		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 Whangee_tunicamycin_UbP		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 Whangee_tunicamycin_WCL		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 Whangee_tunicamycin_WCLP		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.
LFQ intensity Apubscrawl_Cerulenin_Ub		
LFQ intensity Apubscrawl_Cerulenin_UbP		
LFQ intensity Apubscrawl_Cerulenin_WCL		
LFQ intensity Apubscrawl_Cerulenin_WCLP		
LFQ intensity Apubscrawl_Swe1KO_Ub		
LFQ intensity Apubscrawl_Swe1KO_UbP		
LFQ intensity Apubscrawl_Swe1KO_WCL		
LFQ intensity Apubscrawl_Swe1KO_WCLP		
LFQ intensity Control_Ub		
LFQ intensity Control_UbP		
LFQ intensity Control_WCL		
LFQ intensity Control_WCLP		
LFQ intensity EtOH_Kin3KO_Ub		
LFQ intensity EtOH_Kin3KO_UbP		
LFQ intensity EtOH_Kin3KO_WCL		
LFQ intensity EtOH_Kin3KO_WCLP		
LFQ intensity EtOH_menadione_Ub		
LFQ intensity EtOH_menadione_UbP		
LFQ intensity EtOH_menadione_WCL		
LFQ intensity EtOH_menadione_WCLP		
LFQ intensity Onion_Atg1KO_Ub		
LFQ intensity Onion_Atg1KO_UbP		
LFQ intensity Onion_Atg1KO_WCL		
LFQ intensity Onion_Atg1KO_WCLP		
LFQ intensity Onion_rapamycin_Ub		
LFQ intensity Onion_rapamycin_UbP		
LFQ intensity Onion_rapamycin_WCL		
LFQ intensity Onion_rapamycin_WCLP		
LFQ intensity Pynd_5FC_Ub		
LFQ intensity Pynd_5FC_UbP		
LFQ intensity Pynd_5FC_WCL		
LFQ intensity Pynd_5FC_WCLP		
LFQ intensity Pynd_AlkKO_Ub		
LFQ intensity Pynd_AlkKO_UbP		
LFQ intensity Pynd_AlkKO_WCL		
LFQ intensity Pynd_AlkKO_WCLP		

LFQ intensity Shmoo_CaCl2_Ub		
LFQ intensity Shmoo_CaCl2_WCL		
LFQ intensity Shmoo_Cmk1KO_Ub		
LFQ intensity Shmoo_Cmk1KO_UbP		
LFQ intensity Shmoo_Cmk1KO_WCL		
LFQ intensity Shmoo_Cmk1KO_WCLP		
LFQ intensity Whangee_Tpk1KO_Ub		
LFQ intensity Whangee_Tpk1KO_UbP		
LFQ intensity Whangee_Tpk1KO_WCL		
LFQ intensity Whangee_Tpk1KO_WCLP		
LFQ intensity Whangee_tunicamycin_Ub		
LFQ intensity Whangee_tunicamycin_UbP		
LFQ intensity Whangee_tunicamycin_WCL		
LFQ intensity Whangee_tunicamycin_WCLP		
MS/MS Count Apubscrawl_Cerulenin_Ub		
MS/MS Count Apubscrawl_Cerulenin_UbP		
MS/MS Count Apubscrawl_Cerulenin_WCL		
MS/MS Count Apubscrawl_Cerulenin_WCLP		
MS/MS Count Apubscrawl_Swe1KO_Ub		
MS/MS Count Apubscrawl_Swe1KO_UbP		
MS/MS Count Apubscrawl_Swe1KO_WCL		
MS/MS Count Apubscrawl_Swe1KO_WCLP		
MS/MS Count Control_Ub		
MS/MS Count Control_UbP		
MS/MS Count Control_WCL		
MS/MS Count Control_WCLP		
MS/MS Count EtOH_Kin3KO_Ub		
MS/MS Count EtOH_Kin3KO_UbP		
MS/MS Count EtOH_Kin3KO_WCL		
MS/MS Count EtOH_Kin3KO_WCLP		
MS/MS Count EtOH_menadione_Ub		
MS/MS Count EtOH_menadione_UbP		
MS/MS Count EtOH_menadione_WCL		
MS/MS Count EtOH_menadione_WCLP		
MS/MS Count Onion_Atg1KO_Ub		
MS/MS Count Onion_Atg1KO_UbP		
MS/MS Count Onion_Atg1KO_WCL		
MS/MS Count Onion_Atg1KO_WCLP		
MS/MS Count Onion_rapamycin_Ub		
MS/MS Count Onion_rapamycin_UbP		
MS/MS Count Onion_rapamycin_WCL		
MS/MS Count Onion_rapamycin_WCLP		
MS/MS Count Pynd_5FC_Ub		
MS/MS Count Pynd_5FC_UbP		

MS/MS Count Pynd_5FC_WCL		
MS/MS Count Pynd_5FC_WCLP		
MS/MS Count Pynd_AIkKO_Ub		
MS/MS Count Pynd_AIkKO_UbP		
MS/MS Count Pynd_AIkKO_WCL		
MS/MS Count Pynd_AIkKO_WCLP		
MS/MS Count Shmoo_CaCl2_Ub		
MS/MS Count Shmoo_CaCl2_WCL		
MS/MS Count Shmoo_Cmk1KO_Ub		
MS/MS Count Shmoo_Cmk1KO_UbP		
MS/MS Count Shmoo_Cmk1KO_WCL		
MS/MS Count Shmoo_Cmk1KO_WCLP		
MS/MS Count Whangee_Tpk1KO_Ub		
MS/MS Count Whangee_Tpk1KO_UbP		
MS/MS Count Whangee_Tpk1KO_WCL		
MS/MS Count Whangee_Tpk1KO_WCLP		
MS/MS Count Whangee_tunicamycin_Ub		
MS/MS Count Whangee_tunicamycin_UbP		
MS/MS Count Whangee_tunicamycin_WCL		
MS/MS Count Whangee_tunicamycin_WCLP		
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.
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.
Phospho (STY) 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 positions		Positions of the sites in the leading protein of this group.
Phospho (STY) site positions		Positions of the sites in the leading protein of this group.

# All peptides

Name	Separator	Description
Raw file		Name of the raw file the spectral data was extracted from.
Type		The type of detection for the peptide. MULTI – A labeling multiplet was detected. ISO – An isotope pattern was detected.
Charge		The charge state of the peptide.
m/z		The mass divided by the charge of the charged peptide.
Mass		The mass of the neutral peptide ((m/z-proton) * charge).
Uncalibrated m/z		m/z before recalibrations have been applied.
Resolution		The resolution of the peak detected for the peptide measured in Full Width at Half Maximum (FWHM).
Number of data points		The number of data points (peak centroids) collected for this peptide feature.
Number of scans		The number of MS scans that the 3d peaks of this peptide feature are overlapping with.
Number of isotopic peaks		The number of isotopic peaks contained in this peptide feature.
PIF		Short for Parent Ion Fraction; indicates the fraction the target peak makes up of the total intensity in the inclusion window.
Mass fractional part		The values after the radix point (ie value - floor(value)).
Mass deficit		Empirically derived deviation measure to the next nearest integer scaled to center around 0. Can be used to visually detect contaminants in a plot setting Mass against this value.  $m*a+b - \text{round}(m*a+b)$ m: the peptide mass a: 0.999555 b: -0.10
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 timepoint – first timepoint) in seconds.
Retention length (FWHM)		The full width at half maximum value retention time width of the peak in seconds.
Min scan number		The first scan-number at which the peak was encountered.
Max scan number		The last scan-number at which the peak was encountered.
Identified		When marked with '+' this particular MS/MS scan was identified as a peptide; when marked with '-' no identification was made.
MS/MS IDs		Unique identifier linking this identification to the MS/MS scans.
Sequence		The identified AA sequence of the peptide.
Length		The length of the sequence stored in the column "Sequence".
Modifications		Post-translational modifications contained within the sequence. When no modifications exist, this is set to 'unmodified'.  Note: This column only set when this MS/MS spectrum has been identified.
Modified sequence		Sequence representation of the peptide including location(s) of modified AAs.  Note: This column only set when this MS/MS spectrum has been identified.
Proteins		Identifiers of proteins this peptide is associated with.  Note: This column only set when this MS/MS spectrum has been identified.
Score		The score of the identification (higher is better).  Note: This column only set when this MS/MS spectrum has been identified.
Intensity		Summed up eXtracted Ion Current (XIC) of all isotopic clusters associated with the identified AA sequence. In case of a labeled experiment this is the total intensity of all the isotopic patterns in the label cluster.
Intensities		The intensity values of the isotopes.
MS/MS Count		The number of MS/MS spectra recorded for the peptide.

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



# MS scans

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

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

# MZ range

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

# MS/MS scans

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

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

# MS/MS

Name	Separator	Description
Raw file		The name of the RAW file the mass spectral data was read from.
Scan number		The RAW-file derived scan number of the MS/MS spectrum.
Scan index		The consecutive index of the MS/MS spectrum.
Sequence		The identified AA sequence of the peptide.
Length		The length of the sequence stored in the column "Sequence".
Missed cleavages		Number of missed enzymatic cleavages.
Modifications		Post-translational modifications contained within the identified peptide sequence.
Modified sequence		Sequence representation including the post-translational modifications (abbreviation of the modification in brackets before the modified AA). The sequence is always surrounded by underscore characters ('_').
Oxidation (M) Probabilities		Sequence representation of the peptide including PTM positioning probabilities ([0..1], where 1 is best match) for 'Oxidation (M)'.
Phospho (STY) Probabilities		Sequence representation of the peptide including PTM positioning probabilities ([0..1], where 1 is best match) for 'Phospho (STY)'.
Oxidation (M) Score Diffs		
Phospho (STY) Score Diffs		
Acetyl (Protein N-term)		
Oxidation (M)		
Phospho (STY)		
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.
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 ScanNumber		The full scan number where the precursor ion was selected for fragmentation.

Precursor Intensity		The intensity of the precursor ion at the scannumber 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.
Diagnostic peak Phospho (STY) Y		
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		
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'.
Oxidation (M) site IDs		Identifier of the oxidation summary stored in the file 'Oxidation (M)Sites.txt'.
Phospho (STY) site IDs		Identifier of the oxidation summary stored in the file 'Phospho (STY)Sites.txt'.

# AIF MS/MS

Name	Separator	Description
id		A unique (consecutive) identifier for each row in the AIF MS/MS 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 for analyzed peptide evidence associated with the protein group referenced against the evidences table.
Oxidation (M) site IDs		
Phospho (STY) site IDs		
Raw file		Name of the RAW file the spectral data was extracted from, which led to the identification of this peptide.
Sequence		The identified AA sequence of the peptide.
Length		The length of the sequence stored in the column "Sequence".
Missed Cleavages		Number of missed enzymatic cleavages.
Modifications		Post-translational modifications contained within the 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.
Oxidation (M) Probabilities		
Phospho (STY) Probabilities		
Oxidation (M) Score Diffs		
Phospho (STY) Score Diffs		
Acetyl (Protein N-term)		
Oxidation (M)		
Phospho (STY)		
Proteins		The IPI identifiers of the proteins the identified peptide is associated with.
Charge		The charge of the precursor ion.
m/z		The mass-over-charge of the precursor ion.
Mass		The charge corrected mass of the precursor ion.
Retention time		The uncalibrated retention time in minutes in the elution profile of the precursor ion.
Precursor intensity		The intensity of the precursor ion.
PEP		Posterior Error Probability of the identification. This value essentially operates as a p-value, where smaller is more significant.
Score		Andromeda identification score for the 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.
Matches		
Intensities		The intensities of the peaks in the fragmentation spectrum after top-N filtering.
Mass Deviations		The search engine allowed mass deviations of the peaks in the fragmentation spectrum.
Masses		The masses-over-charge of the peaks in the fragmentation spectrum.
Charges		
Correlations		
Number of Matches		
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.