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.
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.
Multiplicity		The number of labels used.
Max. missed cleavages		The maximum allowed number of missed cleavages.
Max. labeled AAs		The maximum allowed of labeled amino acids in a peptide amino acid sequence.
Labels0		The labels used in the labeling experiment. Allowed values for X: 0=light; 1=medium; 2=heavy label partner.
Labels1		The labels used in the labeling experiment. Allowed values for X: 0=light; 1=medium; 2=heavy label partner.
Labels2		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 tandem MS 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.
Multiplets	The total number of detected labeling triplets.
Multiplets z=1	The total number of detected labeling triplets with a charge state of 1.
Multiplets z=2	The total number of detected labeling triplets with a charge state of 2.
Multiplets z=3	The total number of detected labeling triplets with a charge state of 3.
Multiplets z=4	The total number of detected labeling triplets with a charge state of 4.
Multiplets z=5	The total number of detected labeling triplets with a charge state of 5.
Multiplets z=6	The total number of detected labeling triplets with a charge state of 6.
Multiplets z=7	The total number of detected labeling triplets with a charge state of 7.
Multiplets z=8	The total number of detected labeling triplets with a charge state of 8.
Multiplets z=9	The total number of detected labeling triplets with a charge state of 9.
Multiplets z=10	The total number of detected labeling triplets with a charge state of 10.
Multiplets Sequenced	The total number of labeling triplets sequenced by tandem MS.
Multiplets Sequenced [%]	The percentage of labeling triplets sequenced by tandem MS.
Multiplets Repeatedly Sequenced	The total number of labeling triplets repeatedly sequenced (i.e. 1 or more times) by tandem MS.
Multiplets Repeatedly Sequenced [%]	The percentage of labeling triplets repeatedly sequenced (i.e. 1 or more times) by tandem MS.
Multiplets Identified	The total number of labeling triplets identified.
Multiplets Identified [%]	The percentage of labeling triplets identified.
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'.
K Count		The number of instances of K contained within the sequence. The value for this can reliably be determined in the case of labeling partners based on the distance between the partners. These counts are used to solidify the peptide identification process.
R Count		The number of instances of R contained within the sequence. The value for this can reliably be determined in the case of labeling partners based on the distance between the partners. These counts are used to solidify the peptide identification process.
Modifications		Post-translational modifications contained within the identified peptide sequence.
Modified sequence		Sequence representation including the post-translational modifications (abbreviation of the modification in brackets before the modified AA). The sequence is always surrounded by underscore characters ('_').
Deamidation (NQ) Probabilities		Sequence representation of the peptide including PTM positioning probabilities ([01], where 1 is best match) for 'Deamidation (NQ)'.
Oxidation (M) Probabilities		Sequence representation of the peptide including PTM positioning probabilities ([01], where 1 is best match) for 'Oxidation (M)'.
Phospho (S) Probabilities		Sequence representation of the peptide including PTM positioning probabilities ([01], where 1 is best match) for 'Phospho (S)'.
SUMO3 Probabilities		Sequence representation of the peptide including PTM positioning probabilities ([01], where 1 is best match) for 'SUMO3'.
Deamidation (NQ) Score Diffs		Sequence representation for each of the possible PTM positions in each possible configuration, the difference is calculated between the identification score with the PTM added to that position and the best scoring identification where no PTM is added to that position. When this value is negative, it is unlikely that the particular modification is located at this position.
Oxidation (M) Score Diffs		Sequence representation for each of the possible PTM positions in each possible configuration, the difference is calculated between the identification score with the PTM added to that position and the best scoring identification where no PTM is added to that position. When this value is negative, it is unlikely that the particular modification is located at this position.
Phospho (S) 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.
SUMO3 Score Diffs		Sequence representation for each of the possible PTM positions in each possible configuration, the difference is calculated between the identification score with the PTM added to that position and the best scoring identification where no PTM is added to that position. When this value is negative, it is unlikely that the particular modification is located at this position.
Acetyl (Protein N-term)		The number of occurrences of the modification 'Acetyl (Protein N-term)'.
Deamidation (NQ)		The number of occurrences of the modification 'Deamidation (NQ)'.
Oxidation (M)		The number of occurrences of the modification 'Oxidation (M)'.
Phospho (S)		The number of occurrences of the modification 'Phospho (S)'.
SUMO3		The number of occurrences of the modification 'SUMO3'.
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.
Gene Names	Names of genes this peptide is associated with.
Protein Names	Names of proteins this peptide is associated with.
Туре	The type of MS/MS spectrum this sequence is derived from. MSMS – MS/MS for an unidentified peak. ISO-MSMS – MS/MS from an identified isotope cluster. MULTI-MSMS – MS/MS from an identified labeling cluster.
Labeling State	Labeling state of the precursor isotope pattern used to identify the peptide.
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 monoisotopic 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.
Max intensity m/z 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.
Max intensity m/z 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.
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.
Ratio M/L	The ratio between two medium and light label partners.
Ratio M/L normalized	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L shift	The median of the total ratio population was stilled to 1.
Ratio H/L	The ratio between two heavy and light label partners.
Ratio H/L normalized	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L shift	
Ratio H/M	The ratio between two heavy and medium label partners.
Ratio H/M normalized	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M shift	
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 L	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the light label partner.
Intensity M	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the medium label partner.
Intensity H	Summed up eXtracted lon Current (XIC) of the isotopic cluster linked to the heavy label partner.
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'.
Deamidation (NQ) site IDs	Identifier(s) of the modification summary stored in the file 'Deamidation (NQ)Sites.txt'.
Oxidation (M) site IDs	Identifier(s) of the modification summary stored in the file 'Oxidation (M)Sites.txt'.
Phospho (S) site IDs	Identifier(s) of the modification summary stored in the file 'Phospho (S)Sites.txt'.
SUMO3 site IDs	Identifier(s) of the modification summary stored in the file 'SUMO3Sites.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.
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)
Gene names		Names of genes this peptide is associated with.
Protein names		Names of proteins this 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
Chargos	single protein sequence in the fasta file(s). All charge states that have been observed.
PEP 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 C1	Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type C2	Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type C3	Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type N1	Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type N2	Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type N3	Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Experiment C1	Number of evidence entries for this 'Experiment'.
Experiment C2	Number of evidence entries for this 'Experiment'.
Experiment C3	Number of evidence entries for this 'Experiment'.
Experiment N1	Number of evidence entries for this 'Experiment'.
Experiment N2	Number of evidence entries for this 'Experiment'.
Experiment N3	Number of evidence entries for this 'Experiment'.
Ratio M/L	The ratio between two medium and light label partners.
Ratio M/L normalized	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L variability [%]	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio M/L count	Number of redundant peptides (MS1 features) used for quantitation.
Ratio M/L iso-count	Number of redundant peptides (MS1 features) used for guantitation that are quantified with the re-quantify method.
Ratio M/L type	
Ratio H/L	The ratio between two heavy and light label partners.
Ratio H/L normalized	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L variability [%]	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/L count	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/L iso-count	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/L type	
Ratio H/M	The ratio between two heavy and medium label partners.
Ratio H/M normalized	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M variability [%]	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/M count	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/M iso-count	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/M type	
Ratio M/L C1	The ratio between two medium and light label partners.
Ratio M/L normalized C1	The ratio between two medium and light label partners.
Ratio M/L variability [%] C1	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio M/L count C1	Number of redundant peptides (MS1 features) used for quantitation.
Ratio M/L iso-count C1	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio M/L type C1	
Ratio H/L C1	The ratio between two heavy and light label partners.
Ratio H/L normalized C1	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.

Ratio H/L variability [%] C1	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/L count C1	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/L iso-count C1	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/L type C1	
Ratio H/M C1	The ratio between two heavy and medium label partners.
Ratio H/M normalized C1	Normalized ratio between two heavy and medium label
Ratio H/M Hormanzeu CT	partners. The median of the total ratio population was shifted to 1.
Ratio H/M variability [%] C1	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/M count C1	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/M iso-count C1	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/M type C1	
Ratio M/L C2	The ratio between two medium and light label partners.
Ratio M/L normalized C2	The ratio between two medium and light label partners.
Ratio M/L variability [%] C2	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio M/L count C2	Number of redundant peptides (MS1 features) used for quantitation.
Ratio M/L iso-count C2	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio M/L type C2	
Ratio H/L C2	The ratio between two heavy and light label partners.
Ratio H/L normalized C2	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L variability [%] C2	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/L count C2	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/L iso-count C2	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/L type C2	
Ratio H/M C2	The ratio between two heavy and medium label partners.
Ratio H/M normalized C2	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M variability [%] C2	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/M count C2	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/M iso-count C2	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/M type C2	
Ratio M/L C3	The ratio between two medium and light label partners.
Ratio M/L normalized C3	The ratio between two medium and light label partners.
Ratio M/L variability [%] C3	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio M/L count C3	Number of redundant peptides (MS1 features) used for quantitation.
Ratio M/L iso-count C3	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio M/L type C3	
Ratio H/L C3	The ratio between two heavy and light label partners.
Ratio H/L normalized C3	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L variability [%] C3	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/L count C3	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/L iso-count C3	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/L type C3	
Ratio H/M C3	The ratio between two heavy and medium label partners.
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Ratio H/M normalized C3	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M variability [%] C3	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/M count C3	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/M iso-count C3	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/M type C3	
Ratio M/L N1	The ratio between two medium and light label partners.
Ratio M/L normalized N1	The ratio between two medium and light label partners.
Ratio M/L variability [%] N1	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio M/L count N1	Number of redundant peptides (MS1 features) used for quantitation.
Ratio M/L iso-count N1	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio M/L type N1	
Ratio H/L N1	The ratio between two heavy and light label partners.
Ratio H/L normalized N1	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L variability [%] N1	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/L count N1	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/L iso-count N1	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/L type N1	
Ratio H/M N1	The ratio between two heavy and medium label partners.
Ratio H/M normalized N1	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M variability [%] N1	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/M count N1	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/M iso-count N1	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/M type N1	
Ratio M/L N2	The ratio between two medium and light label partners.
Ratio M/L normalized N2	The ratio between two medium and light label partners.
Ratio M/L variability [%] N2	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio M/L count N2	Number of redundant peptides (MS1 features) used for quantitation.
Ratio M/L iso-count N2	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio M/L type N2	
Ratio H/L N2	The ratio between two heavy and light label partners.
Ratio H/L normalized N2	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L variability [%] N2	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/L count N2	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/L iso-count N2	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/L type N2	
Ratio H/M N2	The ratio between two heavy and medium label partners.
Ratio H/M normalized N2	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M variability [%] N2	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/M count N2	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/M iso-count N2	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.

Ratio H/M type N2	
Ratio M/L N3	The ratio between two medium and light label partners.
Ratio M/L normalized N3	The ratio between two medium and light label partners.
Ratio M/L variability [%] N3	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio M/L count N3	Number of redundant peptides (MS1 features) used for quantitation.
Ratio M/L iso-count N3	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio M/L type N3	
Ratio H/L N3	The ratio between two heavy and light label partners.
Ratio H/L normalized N3	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L variability [%] N3	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/L count N3	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/L iso-count N3	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/L type N3	
Ratio H/M N3	The ratio between two heavy and medium label partners.
Ratio H/M normalized N3	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M variability [%] N3	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/M count N3	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/M iso-count N3	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/M type N3	
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 L	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the light label partner.
Intensity M	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the medium label partner.
Intensity H	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the heavy label partner.
Intensity C1	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 L C1	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the light label partner.
Intensity M C1	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the medium label partner.
Intensity H C1	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the heavy label partner.
Intensity C2	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 L C2	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the light label partner.
Intensity M C2	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the medium label partner.
Intensity H C2	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the heavy label partner.
Intensity C3	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 L C3	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the light label partner.
Intensity M C3	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the medium label partner.
Intensity H C3	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the heavy label partner.
Intensity N1	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 L N1	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the light label partner.
Intensity M N1	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the medium label partner.
Intensity H N1	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the heavy label partner.
Intensity N2	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 L N2	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the light label partner.
Intensity M N2	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the medium label partner.
Intensity H N2	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the heavy label partner.
Intensity N3	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 L N3	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the light label partner.
Intensity M N3	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the medium label partner.
Intensity H N3	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the heavy label partner.
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.
Deamidation (NQ) site IDs	Identifier(s) for site(s) associated with the protein group, which show(s) evidence of the modification, referenced against the appropriate modification site file.
Oxidation (M) site IDs	Identifier(s) for site(s) associated with the protein group, which show(s) evidence of the modification, referenced against the appropriate modification site file.
Phospho (S) 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.
SUMO3 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.
K Count		The number of instances of the 'K' AA contained within the sequence. The value for this can reliably be determined in the case of SILAC partners based on the distance between the partners. These counts are used to solidify the peptide identification process.
R Count		The number of instances of the 'R' AA contained within the sequence. The value for this can reliably be determined in the case of SILAC partners based on the distance between the partners. These counts are used to solidify the peptide identification process.
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 whoch this peptide belongs.
Proteins		The identifiers of the proteins this particular peptide is associated with.
Gene Names		Names of genes this peptide is associated with.
Protein Names		Names of proteins this peptide is associated with.
Unique (Groups)		When marked with '+', this particular peptide is unique to a single protein group in the proteinGroups file.
Unique (Proteins)		When marked with '+', this particular peptide is unique to a single protein sequence in the fasta file(s).
Acetyl (Protein N-term)		Number of Acetyl (Protein N-term) on this peptide.
Deamidation (NQ)		Number of Deamidation (NQ) on this peptide.
Oxidation (M)		Number of Oxidation (M) on this peptide.
Phospho (S)		Number of Phospho (S) on this peptide.
SUMO3		Number of SUMO3 on this peptide.
Missed cleavages		Number of missed enzymatic cleavages.
Identification type C1		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type C2		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type C3		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type N1		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type N2		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type N3		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Experiment C1		Number of evidence entries for this 'Experiment'.
Experiment C2		Number of evidence entries for this 'Experiment'.
Experiment C3		Number of evidence entries for this 'Experiment'.
Experiment N1		Number of evidence entries for this 'Experiment'.
Experiment N2		Number of evidence entries for this 'Experiment'.
Experiment N3		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.

Ratio M/L	The ratio between two medium and light label partners.
Ratio M/L normalized	Normalized ratio between two heavy and light label partners.
Ratio M/L variability [%]	The median of the total ratio population was shifted to 1. Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio M/L count	Number of redundant peptides (MS1 features) used for quantitation.
Ratio M/L iso-count	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio M/L type	
Ratio H/L	The ratio between two heavy and light label partners.
Ratio H/L normalized	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L variability [%]	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/L count	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/L iso-count	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/L type	
Ratio H/M	The ratio between two heavy and medium label partners.
Ratio H/M normalized	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M variability [%]	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/M count	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/M iso-count	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/M type	
Ratio M/L C1	The ratio between two medium and light label partners.
Ratio M/L normalized C1	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L variability [%] C1	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio M/L count C1	Number of redundant peptides (MS1 features) used for quantitation.
Ratio M/L iso-count C1	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio M/L type C1	
Ratio H/L C1	The ratio between two heavy and light label partners.
Ratio H/L normalized C1	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L variability [%] C1	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/L count C1	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/L iso-count C1	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/L type C1	
Ratio H/M C1	The ratio between two heavy and medium label partners.
Ratio H/M normalized C1	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M variability [%] C1	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/M count C1	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/M iso-count C1	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/M type C1	
Ratio M/L C2	The ratio between two medium and light label partners.
Ratio M/L normalized C2	Normalized ratio between two heavy and light label partners.
Ratio M/L variability [%] C2	The median of the total ratio population was shifted to 1. Coefficient of variability over all redundant quantifiable
	peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio M/L count C2	Number of redundant peptides (MS1 features) used for quantitation.

Ratio M/L iso-count C2	Number of redundant peptides (MS1 features) used for
	quantitation that are quantified with the re-quantify method.
Ratio M/L type C2	The making between two forestern and Protect Co.
Ratio H/L C2	The ratio between two heavy and light label partners.
Ratio H/L normalized C2	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L variability [%] C2	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/L count C2	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/L iso-count C2	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/L type C2	
Ratio H/M C2	The ratio between two heavy and medium label partners.
Ratio H/M normalized C2	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M variability [%] C2	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/M count C2	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/M iso-count C2	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/M type C2	
Ratio M/L C3	The ratio between two medium and light label partners.
Ratio M/L normalized C3	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L variability [%] C3	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio M/L count C3	Number of redundant peptides (MS1 features) used for quantitation.
Ratio M/L iso-count C3	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio M/L type C3	
Ratio H/L C3	The ratio between two heavy and light label partners.
Ratio H/L normalized C3	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L variability [%] C3	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/L count C3	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/L iso-count C3	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/L type C3	
Ratio H/M C3	The ratio between two heavy and medium label partners.
Ratio H/M normalized C3	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M variability [%] C3	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/M count C3	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/M iso-count C3	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/M type C3	
Ratio M/L N1	The ratio between two medium and light label partners.
Ratio M/L normalized N1	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L variability [%] N1	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio M/L count N1	Number of redundant peptides (MS1 features) used for quantitation.
<u> </u>	
Ratio M/L iso-count N1	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio M/L iso-count N1 Ratio M/L type N1	Number of redundant peptides (MS1 features) used for
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	peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/L count N1	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/L iso-count N1	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/L type N1	
Ratio H/M N1	The ratio between two heavy and medium label partners.
Ratio H/M normalized N1	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M variability [%] N1	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/M count N1	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/M iso-count N1	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/M type N1	
Ratio M/L N2	The ratio between two medium and light label partners.
Ratio M/L normalized N2	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L variability [%] N2	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio M/L count N2	Number of redundant peptides (MS1 features) used for quantitation.
Ratio M/L iso-count N2	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio M/L type N2	
Ratio H/L N2	The ratio between two heavy and light label partners.
Ratio H/L normalized N2	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L variability [%] N2	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/L count N2	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/L iso-count N2	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/L type N2	
Ratio H/M N2	The ratio between two heavy and medium label partners.
Ratio H/M normalized N2	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M variability [%] N2	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/M count N2	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/M iso-count N2	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/M type N2	
Ratio M/L N3	The ratio between two medium and light label partners.
Ratio M/L normalized N3	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L variability [%] N3	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio M/L count N3	Number of redundant peptides (MS1 features) used for quantitation.
Ratio M/L iso-count N3	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio M/L type N3	
Ratio H/L N3	The ratio between two heavy and light label partners.
Ratio H/L normalized N3	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L variability [%] N3	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/L count N3	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/L iso-count N3	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/L type N3	, and provide the second secon
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Ratio H/M N3	The ratio between two heavy and medium label partners.
Ratio H/M normalized N3	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to
Ratio H/M variability [%] N3	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/M count N3	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/M iso-count N3	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/M type N3	
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 L	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the light label partner.
Intensity M	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the medium label partner.
Intensity H	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the heavy label partner.
Intensity C1	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 L C1	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the light label partner.
Intensity M C1	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the medium label partner.
Intensity H C1	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the heavy label partner.
Intensity C2	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 L C2	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the light label partner.
Intensity M C2	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the medium label partner.
Intensity H C2	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the heavy label partner.
Intensity C3	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 L C3	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the light label partner.
Intensity M C3	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the medium label partner.
Intensity H C3	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the heavy label partner.
Intensity N1	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 L N1	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the light label partner.
Intensity M N1	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the medium label partner.
Intensity H N1	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the heavy label partner.
Intensity N2	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 L N2	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the light label partner.
Intensity M N2	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the medium label partner.
Intensity H N2	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the heavy label partner.
Intensity N3	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 L N3	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the light label partner.
	1

Intensity M N3	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the medium label partner.
Intensity H N3	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the heavy label partner.
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.
Deamidation (NQ) site IDs	Identifier(s) for site(s) associated with this peptide, which show(s) evidence of the modification, referenced against the appropriate modification site file.
Oxidation (M) site IDs	Identifier(s) for site(s) associated with this peptide, which show(s) evidence of the modification, referenced against the appropriate modification site file.
Phospho (S) 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.
SUMO3 site IDs	Identifier(s) for site(s) associated with this peptide, which show(s) evidence of the modification, referenced against the appropriate modification site file.
MS/MS Count	

Deamidation (NQ)Sites

Name	Separator	Description
Proteins		Identifiers of proteins this site is associated with.
Positions within proteins		For each protein identifier in the 'Proteins' column you find here the psoition 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.
Protein names		Names of proteins this peptide is associated with.
Gene names		Names of genes 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 C1		
Score diff C1		
PEP C1		
Score C1		
Localization prob C2		
Score diff C2		
PEP C2		
Score C2		
Localization prob C3		
Score diff C3		
PEP C3		
Score C3		
Localization prob N1		
Score diff N1		
PEP N1		
Score N1		
Localization prob N2		
Score diff N2		
PEP N2		
Score N2		
Localization prob N3		
Score diff N3		
PEP N3		
Score N3		
Diagnostic peak		
Number of Deamidation (NQ)		Different numbers of Deamidation (NQ) on peptides that this site is involved in.
Amino acid		
Sequence window		
Modification window		
Peptide window coverage		
Deamidation (NQ) Probabilities		
Deamidation (NQ) Score diffs		
Position in peptide		
Charge		Charge state of the precursor ion.
Mass error [ppm]		Mass error of the recalibrated mass-over-charge value of the precursor ion in comparison to the predicted monoisotopic mass of the identified peptide sequence.
Identification type C1		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type C2		Indicates whether this experiment was identified by MS/MS or only by matching between runs.

Identification type C3	Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type N1	Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type N2	Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type N3	Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Ratio M/L	The ratio between two medium and light label partners.
Ratio M/L1	The ratio between two medium and light label partners.
Ratio M/L2	The ratio between two medium and light label partners.
Ratio M/L3	The ratio between two medium and light label partners.
Ratio M/L normalized	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized1	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized2	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized3	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L unmod. pep.	
Ratio M/L localized	
Ratio M/L nmods	
Ratio M/L variability [%]	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio M/L count	Number of redundant peptides (MS1 features) used for quantitation.
Ratio M/L iso-count	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio M/L type	
Ratio H/L	The ratio between two heavy and light label partners.
Ratio H/L1	The ratio between two heavy and light label partners.
Ratio H/L2	The ratio between two heavy and light label partners.
Ratio H/L3	The ratio between two heavy and light label partners.
Ratio H/L normalized	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized1	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized2	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized3	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L unmod. pep.	
Ratio H/L localized	
Ratio H/L nmods	
Ratio H/L variability [%]	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/L type	
Ratio H/L count	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/L iso-count	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/M	The ratio between two heavy and medium label partners.
Ratio H/M1	The ratio between two heavy and medium label partners.
Ratio H/M2	The ratio between two heavy and medium label partners.
Ratio H/M3	The ratio between two heavy and medium label partners.
Ratio H/M normalized	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized1	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized2	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized3	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M unmod. pep.	
Ratio H/M localized	
Ratio H/M nmods	

Ratio H/M variability [%]	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/M count	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/M iso-count	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/M type	
Occupancy L	
Occupancy M	
Occupancy H	
Ratio M/L C1	The ratio between two medium and light label partners.
Ratio M/L C11	The ratio between two medium and light label partners.
Ratio M/L C12	The ratio between two medium and light label partners.
Ratio M/L C13	The ratio between two medium and light label partners.
Ratio M/L normalized C1	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized C11	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized C12	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized C13	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L unmod. pep. C1	
Ratio M/L localized C1	
Ratio M/L nmods C1	
Ratio M/L variability [%] C1	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio M/L count C1	Number of redundant peptides (MS1 features) used for quantitation.
Ratio M/L iso-count C1	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio M/L type C1	
Ratio H/L C1	The ratio between two heavy and light label partners.
Ratio H/L C11	The ratio between two heavy and light label partners.
Ratio H/L C12	The ratio between two heavy and light label partners.
Ratio H/L C13	The ratio between two heavy and light label partners.
Ratio H/L normalized C1	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized C11	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized C12	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized C13	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L unmod. pep. C1	
Ratio H/L localized C1	
Ratio H/L nmods C1	
Ratio H/L variability [%] C1	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/L count C1	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/L iso-count C1	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/L type C1	
Ratio H/M C1	The ratio between two heavy and medium label partners.
Ratio H/M C11	The ratio between two heavy and medium label partners.
Ratio H/M C12	The ratio between two heavy and medium label partners.
Ratio H/M C13	The ratio between two heavy and medium label partners.
Ratio H/M normalized C1	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized C11	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized C12	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized C13	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.

Ratio H/M unmod. pep. C1	
Ratio H/M localized C1	
Ratio H/M nmods C1	
Ratio H/M variability [%] C1	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the
Ratio H/M count C1	naturally logarithmized ratios times 100. Number of redundant peptides (MS1 features) used for
Ratio H/M iso-count C1	quantitation. Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/M type C1	
Occupancy L C1	
Occupancy M C1	
Occupancy H C1	
Ratio M/L C2	The ratio between two medium and light label partners.
Ratio M/L C21	The ratio between two medium and light label partners.
Ratio M/L C22	The ratio between two medium and light label partners.
Ratio M/L C2 3	The ratio between two medium and light label partners.
Ratio M/L normalized C2	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized C21	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized C22	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized C23	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L unmod. pep. C2	
Ratio M/L localized C2	
Ratio M/L nmods C2	
Ratio M/L variability [%] C2	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio M/L count C2	Number of redundant peptides (MS1 features) used for quantitation.
Ratio M/L iso-count C2	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio M/L type C2	
Ratio H/L C2	The ratio between two heavy and light label partners.
Ratio H/L C21	The ratio between two heavy and light label partners.
Ratio H/L C22	The ratio between two heavy and light label partners.
Ratio H/L C23	The ratio between two heavy and light label partners.
Ratio H/L normalized C2	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized C21 Ratio H/L normalized C22	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1. Normalized ratio between two medium and light label partners.
Ratio H/L normalized C22 Ratio H/L normalized C2 3	The median of the total ratio population was shifted to 1. Normalized ratio between two medium and light label partners.
Ratio H/L unmod. pep. C2	The median of the total ratio population was shifted to 1.
Ratio H/L localized C2	
Ratio H/L nmods C2	
Ratio H/L variability [%] C2	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the
Ratio H/L count C2	naturally logarithmized ratios times 100. Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/L iso-count C2	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/L type C2	
Ratio H/M C2	The ratio between two heavy and medium label partners.
Ratio H/M C21	The ratio between two heavy and medium label partners.
Ratio H/M C22	The ratio between two heavy and medium label partners.
Ratio H/M C23	The ratio between two heavy and medium label partners.
Ratio H/M normalized C2	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized C21	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.

Ratio H/M normalized C22	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized C23	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M unmod. pep. C2	
Ratio H/M localized C2	
Ratio H/M nmods C2	
Ratio H/M variability [%] C2	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/M count C2	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/M iso-count C2	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/M type C2	
Occupancy L C2	
Occupancy M C2	
Occupancy H C2	
Ratio M/L C3	The ratio between two medium and light label partners.
Ratio M/L C3 1	The ratio between two medium and light label partners.
Ratio M/L C3 2	The ratio between two medium and light label partners.
Ratio M/L C3 3	The ratio between two medium and light label partners.
Ratio M/L normalized C3	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized C31	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized C32	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized C33	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L unmod. pep. C3	·
Ratio M/L localized C3	
Ratio M/L nmods C3	
Ratio M/L variability [%] C3	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio M/L count C3	Number of redundant peptides (MS1 features) used for quantitation.
Ratio M/L iso-count C3	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio M/L type C3	
Ratio H/L C3	The ratio between two heavy and light label partners.
Ratio H/L C31	The ratio between two heavy and light label partners.
Ratio H/L C32	The ratio between two heavy and light label partners.
Ratio H/L C33	The ratio between two heavy and light label partners.
Ratio H/L normalized C3	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized C31	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized C32	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized C33	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L unmod. pep. C3	
Ratio H/L localized C3	
Ratio H/L nmods C3	
Ratio H/L variability [%] C3	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/L count C3	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/L iso-count C3	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/L type C3	
Ratio H/M C3	The ratio between two heavy and medium label partners.
Ratio H/M C31	The ratio between two heavy and medium label partners.
Ratio H/M C32	The ratio between two heavy and medium label partners.

Ratio H/M normalized C3	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to
	1.
Ratio H/M normalized C31	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized C32	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized C33	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M unmod. pep. C3	
Ratio H/M localized C3	
Ratio H/M nmods C3	
Ratio H/M variability [%] C3	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/M count C3	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/M iso-count C3	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/M type C3	
Occupancy L C3	
Occupancy M C3	
Occupancy H C3	
Ratio M/L N1	The ratio between two medium and light label partners.
Ratio M/L N11	The ratio between two medium and light label partners.
Ratio M/L N12	The ratio between two medium and light label partners.
Ratio M/L N13	The ratio between two medium and light label partners.
Ratio M/L normalized N1	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized N11	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized N12	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized N13	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L unmod. pep. N1	
Ratio M/L localized N1	
Ratio M/L nmods N1	
Ratio M/L variability [%] N1	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio M/L count N1	Number of redundant peptides (MS1 features) used for quantitation.
Ratio M/L iso-count N1	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio M/L type N1	
Ratio H/L N1	The ratio between two heavy and light label partners.
Ratio H/L N11	The ratio between two heavy and light label partners.
Ratio H/L N12	The ratio between two heavy and light label partners.
Ratio H/L N13	The ratio between two heavy and light label partners.
Ratio H/L normalized N1	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized N11	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized N12	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized N13	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L unmod. pep. N1	
Ratio H/L localized N1	
Ratio H/L nmods N1	
Ratio H/L variability [%] N1	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/L count N1	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/L iso-count N1	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/L type N1	
Ratio H/M N1	The ratio between two heavy and medium label partners.

Ratio H/M N11	The ratio between two heavy and medium label partners.
Ratio H/M N12	The ratio between two heavy and medium label partners.
Ratio H/M N13	The ratio between two heavy and medium label partners.
Ratio H/M normalized N1	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized N11	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to
Ratio H/M normalized N12	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized N13	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M unmod. pep. N1	
Ratio H/M localized N1	
Ratio H/M nmods N1	
Ratio H/M variability [%] N1	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/M count N1	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/M iso-count N1	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/M type N1	
Occupancy L N1	
Occupancy M N1	
Occupancy H N1	
Ratio M/L N2	The ratio between two medium and light label partners.
Ratio M/L N21	The ratio between two medium and light label partners.
Ratio M/L N22	The ratio between two medium and light label partners.
Ratio M/L N23	The ratio between two medium and light label partners.
Ratio M/L normalized N2	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized N21	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized N22	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized N23	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L unmod. pep. N2	
Ratio M/L localized N2	
Ratio M/L nmods N2	
Ratio M/L variability [%] N2	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio M/L count N2	Number of redundant peptides (MS1 features) used for quantitation.
Ratio M/L iso-count N2	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio M/L type N2	
Ratio H/L N2	The ratio between two heavy and light label partners.
Ratio H/L N21	The ratio between two heavy and light label partners.
Ratio H/L N22	The ratio between two heavy and light label partners.
Ratio H/L N23	The ratio between two heavy and light label partners.
Ratio H/L normalized N2	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized N21	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized N22	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized N23	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L unmod. pep. N2	
Ratio H/L localized N2	
Ratio H/L nmods N2	
Ratio H/L variability [%] N2	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/L count N2	Number of redundant peptides (MS1 features) used for quantitation.
	- · ·

Ratio H/L iso-count N2	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/L type N2	
Ratio H/M N2	The ratio between two heavy and medium label partners.
Ratio H/M N2 1	The ratio between two heavy and medium label partners.
Ratio H/M N2 2	The ratio between two heavy and medium label partners.
Ratio H/M N2 3	The ratio between two heavy and medium label partners.
	<u> </u>
Ratio H/M normalized N2	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized N21	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized N22	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized N23	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M unmod. pep. N2	
Ratio H/M localized N2	
Ratio H/M nmods N2	
Ratio H/M variability [%] N2	Coefficient of variability over all redundant quantifiable
,,,	peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/M count N2	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/M iso-count N2	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/M type N2	
Occupancy L N2	
Occupancy M N2	
Occupancy H N2	
Ratio M/L N3	The ratio between two medium and light label partners.
Ratio M/L N31	The ratio between two medium and light label partners.
Ratio M/L N32	The ratio between two medium and light label partners.
Ratio M/L N3 3	The ratio between two medium and light label partners.
Ratio M/L normalized N3	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized N31	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized N32	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized N33	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L unmod. pep. N3	
Ratio M/L localized N3	
Ratio M/L nmods N3	
Ratio M/L variability [%] N3	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio M/L count N3	Number of redundant peptides (MS1 features) used for quantitation.
Ratio M/L iso-count N3	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio M/L type N3	
Ratio H/L N3	The ratio between two heavy and light label partners.
Ratio H/L N31	The ratio between two heavy and light label partners.
Ratio H/L N32	The ratio between two heavy and light label partners.
Ratio H/L N33	The ratio between two heavy and light label partners.
Ratio H/L normalized N3	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized N31	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized N32	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized N33	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
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Ratio H/L unmod. pep. N3	
Ratio H/L unmod. pep. N3 Ratio H/L localized N3	

Ratio H/L variability [%] N3	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/L count N3	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/L iso-count N3	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/L type N3	
Ratio H/M N3	The ratio between two heavy and medium label partners.
Ratio H/M N3 1	The ratio between two heavy and medium label partners.
Ratio H/M N3 2	The ratio between two heavy and medium label partners.
Ratio H/M N3 3	The ratio between two heavy and medium label partners.
Ratio H/M normalized N3	Normalized ratio between two heavy and medium label
Ratio 17/W Hormalized NS	partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized N31	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized N32	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized N33	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M unmod. pep. N3	
Ratio H/M localized N3	
Ratio H/M nmods N3	
Ratio H/M variability [%] N3	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/M count N3	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/M iso-count N3	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/M type N3	
Occupancy L N3	
Occupancy M N3	
Occupancy H N3	
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 L	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the light label partner.
Intensity M	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the medium label partner.
Intensity H	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the heavy label partner.
Ratio mod/base L	
Ratio mod/base M	
Ratio mod/base H	
Intensity C1	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 L C1	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the light label partner.
Intensity M C1	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the medium label partner.
Intensity H C1	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the heavy label partner.
Ratio mod/base L C1	
Ratio mod/base M C1	
Ratio mod/base H C1	
Intensity C2	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 L C2	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the light label partner.
Intensity M C2	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the medium label partner.
Intensity H C2	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the heavy label partner.
Ratio mod/base L C2	

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Ratio mod/base M C2	
Ratio mod/base H C2	
Intensity C3	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 L C3	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the light label partner.
Intensity M C3	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the medium label partner.
Intensity H C3	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the heavy label partner.
Ratio mod/base L C3	
Ratio mod/base M C3	
Ratio mod/base H C3	
Intensity N1	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 L N1	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the light label partner.
Intensity M N1	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the medium label partner.
Intensity H N1	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the heavy label partner.
Ratio mod/base L N1	
Ratio mod/base M N1	
Ratio mod/base H N1	
Intensity N2	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 L N2	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the light label partner.
Intensity M N2	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the medium label partner.
Intensity H N2	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the heavy label partner.
Ratio mod/base L N2	
Ratio mod/base M N2	
Ratio mod/base H N2	
Intensity N3	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 L N3	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the light label partner.
Intensity M N3	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the medium label partner.
Intensity H N3	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the heavy label partner.
Ratio mod/base L N3	
Ratio mod/base M N3	
Ratio mod/base H N3	
Occupancy C1	
Occupancy ratioC1	
Occupancy error scale C1	
Occupancy C2	
Occupancy ratioC2	
Occupancy error scale C2	
Occupancy C3	
Occupancy ratioC3	
Occupancy error scale C3	
Occupancy N1	
Occupancy ratioN1	
Occupancy error scale N1	
Occupancy N2	
ia	
Occupancy ratioN2	
Occupancy ratioN2 Occupancy error scale N2	
' '	
Occupancy error scale N2	

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
Potential contaminant	analysis. 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	

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 psoition 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.
Protein names		Names of proteins this peptide is associated with.
Gene names		Names of genes 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 C1		
Score diff C1		
PEP C1		
Score C1		
Localization prob C2		
Score diff C2		
PEP C2		
Score C2		
Localization prob C3		
Score diff C3		
PEP C3		
Score C3		
Localization prob N1		
Score diff N1		
PEP N1		
Score N1		
Localization prob N2		
Score diff N2		
PEP N2		
Score N2		
Localization prob N3		
Score diff N3		
PEP N3		
Score N3		
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 C1		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type C2		Indicates whether this experiment was identified by MS/MS or only by matching between runs.

Identification type C3	Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type N1	Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type N2	Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type N3	Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Ratio M/L	The ratio between two medium and light label partners.
Ratio M/L1	The ratio between two medium and light label partners.
Ratio M/L2	The ratio between two medium and light label partners.
Ratio M/L3	The ratio between two medium and light label partners.
Ratio M/L normalized	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized1	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized2	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized3	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L unmod. pep.	
Ratio M/L localized	
Ratio M/L nmods	
Ratio M/L variability [%]	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio M/L count	Number of redundant peptides (MS1 features) used for quantitation.
Ratio M/L iso-count	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio M/L type	
Ratio H/L	The ratio between two heavy and light label partners.
Ratio H/L1	The ratio between two heavy and light label partners.
Ratio H/L2	The ratio between two heavy and light label partners.
Ratio H/L3	The ratio between two heavy and light label partners.
Ratio H/L normalized	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized1	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized2	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized3	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L unmod. pep.	
Ratio H/L localized	
Ratio H/L nmods	
Ratio H/L variability [%]	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/L type	
Ratio H/L count	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/L iso-count	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/M	The ratio between two heavy and medium label partners.
Ratio H/M1	The ratio between two heavy and medium label partners.
Ratio H/M2	The ratio between two heavy and medium label partners.
Ratio H/M3	The ratio between two heavy and medium label partners.
Ratio H/M normalized	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized1	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized2	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized3	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M unmod. pep.	
Ratio H/M localized	
Ratio H/M nmods	

Ratio H/M variability [%]	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/M count	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/M iso-count	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/M type	
Occupancy L	
Occupancy M	
Occupancy H	
Ratio M/L C1	The ratio between two medium and light label partners.
Ratio M/L C11	The ratio between two medium and light label partners.
Ratio M/L C12	The ratio between two medium and light label partners.
Ratio M/L C13	The ratio between two medium and light label partners.
Ratio M/L normalized C1	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized C11	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized C12	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized C13	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L unmod. pep. C1	
Ratio M/L localized C1	
Ratio M/L nmods C1	
Ratio M/L variability [%] C1	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio M/L count C1	Number of redundant peptides (MS1 features) used for quantitation.
Ratio M/L iso-count C1	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio M/L type C1	
Ratio H/L C1	The ratio between two heavy and light label partners.
Ratio H/L C11	The ratio between two heavy and light label partners.
Ratio H/L C12	The ratio between two heavy and light label partners.
Ratio H/L C13	The ratio between two heavy and light label partners.
Ratio H/L normalized C1	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized C11	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized C12	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized C13	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L unmod. pep. C1	
Ratio H/L localized C1	
Ratio H/L nmods C1	
Ratio H/L variability [%] C1	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/L count C1	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/L iso-count C1	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/L type C1	
Ratio H/M C1	The ratio between two heavy and medium label partners.
Ratio H/M C11	The ratio between two heavy and medium label partners.
Ratio H/M C12	The ratio between two heavy and medium label partners.
Ratio H/M C13	The ratio between two heavy and medium label partners.
Ratio H/M normalized C1	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized C11	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized C12	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized C13	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.

Ratio H/M unmod. pep. C1	
Ratio H/M localized C1	
Ratio H/M nmods C1	
Ratio H/M variability [%] C1	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the
Ratio H/M count C1	naturally logarithmized ratios times 100. Number of redundant peptides (MS1 features) used for
Ratio H/M iso-count C1	quantitation. Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/M type C1	
Occupancy L C1	
Occupancy M C1	
Occupancy H C1	
Ratio M/L C2	The ratio between two medium and light label partners.
Ratio M/L C21	The ratio between two medium and light label partners.
Ratio M/L C22	The ratio between two medium and light label partners.
Ratio M/L C2 3	The ratio between two medium and light label partners.
Ratio M/L normalized C2	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized C21	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized C22	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized C23	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L unmod. pep. C2	
Ratio M/L localized C2	
Ratio M/L nmods C2	
Ratio M/L variability [%] C2	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio M/L count C2	Number of redundant peptides (MS1 features) used for quantitation.
Ratio M/L iso-count C2	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio M/L type C2	
Ratio H/L C2	The ratio between two heavy and light label partners.
Ratio H/L C21	The ratio between two heavy and light label partners.
Ratio H/L C22	The ratio between two heavy and light label partners.
Ratio H/L C23	The ratio between two heavy and light label partners.
Ratio H/L normalized C2	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized C21 Ratio H/L normalized C22	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1. Normalized ratio between two medium and light label partners.
Ratio H/L normalized C22 Ratio H/L normalized C2 3	The median of the total ratio population was shifted to 1. Normalized ratio between two medium and light label partners.
Ratio H/L unmod. pep. C2	The median of the total ratio population was shifted to 1.
Ratio H/L localized C2	
Ratio H/L nmods C2	
Ratio H/L variability [%] C2	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the
Ratio H/L count C2	naturally logarithmized ratios times 100. Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/L iso-count C2	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/L type C2	
Ratio H/M C2	The ratio between two heavy and medium label partners.
Ratio H/M C21	The ratio between two heavy and medium label partners.
Ratio H/M C22	The ratio between two heavy and medium label partners.
Ratio H/M C23	The ratio between two heavy and medium label partners.
Ratio H/M normalized C2	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized C21	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.

Ratio H/M normalized C22	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized C23	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M unmod. pep. C2	
Ratio H/M localized C2	
Ratio H/M nmods C2	
Ratio H/M variability [%] C2	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/M count C2	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/M iso-count C2	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/M type C2	
Occupancy L C2	
Occupancy M C2	
Occupancy H C2	
Ratio M/L C3	The ratio between two medium and light label partners.
Ratio M/L C3 1	The ratio between two medium and light label partners.
Ratio M/L C3 2	The ratio between two medium and light label partners.
Ratio M/L C3 3	The ratio between two medium and light label partners.
Ratio M/L normalized C3	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized C31	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized C32	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized C33	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L unmod. pep. C3	·
Ratio M/L localized C3	
Ratio M/L nmods C3	
Ratio M/L variability [%] C3	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio M/L count C3	Number of redundant peptides (MS1 features) used for quantitation.
Ratio M/L iso-count C3	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio M/L type C3	
Ratio H/L C3	The ratio between two heavy and light label partners.
Ratio H/L C31	The ratio between two heavy and light label partners.
Ratio H/L C32	The ratio between two heavy and light label partners.
Ratio H/L C33	The ratio between two heavy and light label partners.
Ratio H/L normalized C3	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized C31	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized C32	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized C33	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L unmod. pep. C3	
Ratio H/L localized C3	
Ratio H/L nmods C3	
Ratio H/L variability [%] C3	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/L count C3	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/L iso-count C3	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/L type C3	
Ratio H/M C3	The ratio between two heavy and medium label partners.
Ratio H/M C31	The ratio between two heavy and medium label partners.
Ratio H/M C32	The ratio between two heavy and medium label partners.

Ratio H/M normalized C3	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to
	1.
Ratio H/M normalized C31	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized C32	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized C33	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M unmod. pep. C3	
Ratio H/M localized C3	
Ratio H/M nmods C3	
Ratio H/M variability [%] C3	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/M count C3	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/M iso-count C3	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/M type C3	
Occupancy L C3	
Occupancy M C3	
Occupancy H C3	
Ratio M/L N1	The ratio between two medium and light label partners.
Ratio M/L N11	The ratio between two medium and light label partners.
Ratio M/L N12	The ratio between two medium and light label partners.
Ratio M/L N13	The ratio between two medium and light label partners.
Ratio M/L normalized N1	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized N11	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized N12	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized N13	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L unmod. pep. N1	
Ratio M/L localized N1	
Ratio M/L nmods N1	
Ratio M/L variability [%] N1	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio M/L count N1	Number of redundant peptides (MS1 features) used for quantitation.
Ratio M/L iso-count N1	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio M/L type N1	
Ratio H/L N1	The ratio between two heavy and light label partners.
Ratio H/L N11	The ratio between two heavy and light label partners.
Ratio H/L N12	The ratio between two heavy and light label partners.
Ratio H/L N13	The ratio between two heavy and light label partners.
Ratio H/L normalized N1	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized N11	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized N12	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized N13	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L unmod. pep. N1	
Ratio H/L localized N1	
Ratio H/L nmods N1	
Ratio H/L variability [%] N1	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/L count N1	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/L iso-count N1	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/L type N1	
Ratio H/M N1	The ratio between two heavy and medium label partners.

Ratio H/M N11	The ratio between two heavy and medium label partners.
Ratio H/M N12	The ratio between two heavy and medium label partners.
Ratio H/M N13	The ratio between two heavy and medium label partners.
Ratio H/M normalized N1	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized N11	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized N12	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized N13	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M unmod. pep. N1	
Ratio H/M localized N1	
Ratio H/M nmods N1	
Ratio H/M variability [%] N1	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/M count N1	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/M iso-count N1	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/M type N1	
Occupancy L N1	
Occupancy M N1	
Occupancy H N1	
Ratio M/L N2	The ratio between two medium and light label partners.
Ratio M/L N21	The ratio between two medium and light label partners.
Ratio M/L N2 2	The ratio between two medium and light label partners.
Ratio M/L N2 3	The ratio between two medium and light label partners.
Ratio M/L normalized N2	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized N21	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized N22	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized N23	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L unmod. pep. N2	
Ratio M/L localized N2	
Ratio M/L nmods N2	
Ratio M/L variability [%] N2	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio M/L count N2	Number of redundant peptides (MS1 features) used for quantitation.
Ratio M/L iso-count N2	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio M/L type N2	
Ratio H/L N2	The ratio between two heavy and light label partners.
Ratio H/L N21	The ratio between two heavy and light label partners.
Ratio H/L N22	The ratio between two heavy and light label partners.
Ratio H/L N23	The ratio between two heavy and light label partners.
Ratio H/L normalized N2	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized N21	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized N22	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized N23	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L unmod. pep. N2	
Ratio H/L localized N2	
Ratio H/L nmods N2	
Ratio H/L variability [%] N2	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the
	naturally logarithmized ratios times 100.

Ratio H/L iso-count N2	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/L type N2	
Ratio H/M N2	The ratio between two heavy and medium label partners.
Ratio H/M N2 1	The ratio between two heavy and medium label partners.
Ratio H/M N2 2	The ratio between two heavy and medium label partners.
Ratio H/M N2 3	The ratio between two heavy and medium label partners.
Ratio H/M normalized N2	
Ratio H/M normalized Nz	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized N21	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized N22	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized N23	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M unmod. pep. N2	
Ratio H/M localized N2	
Ratio H/M nmods N2	
Ratio H/M variability [%] N2	Coefficient of variability over all redundant quantifiable
	peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/M count N2	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/M iso-count N2	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/M type N2	
Occupancy L N2	
Occupancy M N2	
Occupancy H N2	
Ratio M/L N3	The ratio between two medium and light label partners.
Ratio M/L N31	The ratio between two medium and light label partners.
Ratio M/L N32	The ratio between two medium and light label partners.
Ratio M/L N3 3	The ratio between two medium and light label partners.
Ratio M/L normalized N3	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized N31	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized N32	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized N33	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L unmod. pep. N3	
Ratio M/L localized N3	
Ratio M/L nmods N3	
Ratio M/L variability [%] N3	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio M/L count N3	Number of redundant peptides (MS1 features) used for quantitation.
Ratio M/L iso-count N3	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio M/L type N3	
Ratio H/L N3	The ratio between two heavy and light label partners.
Ratio H/L N31	The ratio between two heavy and light label partners.
Ratio H/L N32	The ratio between two heavy and light label partners.
Ratio H/L N33	The ratio between two heavy and light label partners.
Ratio H/L normalized N3	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized N31	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized N32	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized N33	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L unmod. pep. N3	
Ratio H/L localized N3	

Ratio H/L variability [%] N3	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/L count N3	Number of redundant peptides (MS1 features) used for guantitation.
Ratio H/L iso-count N3	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/L type N3	
Ratio H/M N3	The ratio between two heavy and medium label partners.
Ratio H/M N3 1	The ratio between two heavy and medium label partners.
Ratio H/M N3 2	The ratio between two heavy and medium label partners.
Ratio H/M N3 3	The ratio between two heavy and medium label partners.
Ratio H/M normalized N3	Normalized ratio between two heavy and medium label
Ratio 17/W Hormalized NS	partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized N31	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized N32	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized N33	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M unmod. pep. N3	
Ratio H/M localized N3	
Ratio H/M nmods N3	
Ratio H/M variability [%] N3	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/M count N3	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/M iso-count N3	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/M type N3	
Occupancy L N3	
Occupancy M N3	
Occupancy H N3	
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 L	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the light label partner.
Intensity M	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the medium label partner.
Intensity H	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the heavy label partner.
Ratio mod/base L	
Ratio mod/base M	
Ratio mod/base H	
Intensity C1	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 L C1	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the light label partner.
Intensity M C1	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the medium label partner.
Intensity H C1	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the heavy label partner.
Ratio mod/base L C1	
Ratio mod/base M C1	
Ratio mod/base H C1	
Intensity C2	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 L C2	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the light label partner.
Intensity M C2	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the medium label partner.
Intensity H C2	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the heavy label partner.
Ratio mod/base L C2	

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sequence is the extended t'. roteins (e.g. in e stored here
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des, the same id

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 (S)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 psoition 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.
Protein names		Names of proteins this peptide is associated with.
Gene names		Names of genes 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 C1		
Score diff C1		
PEP C1		
Score C1		
Localization prob C2		
Score diff C2		
PEP C2		
Score C2		
Localization prob C3		
Score diff C3		
PEP C3		
Score C3		
Localization prob N1		
Score diff N1		
PEP N1		
Score N1		
Localization prob N2		
Score diff N2		
PEP N2		
Score N2		
Localization prob N3		
Score diff N3		
PEP N3		+
Score N3		
Diagnostic peak		
Number of Phospho (S)		Different numbers of Phospho (S) on peptides that this site is involved in.
Amino acid		
Sequence window		
Modification window		
Peptide window coverage		
Phospho (S) Probabilities		
Phospho (S) 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
ινιασο σποι [μμπ]		precursor ion in comparison to the predicted monoisotopic mass of the identified peptide sequence.
Identification type C1		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type C2		Indicates whether this experiment was identified by MS/MS or only by matching between runs.

Identification type C3	Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type N1	Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type N2	Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type N3	Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Ratio M/L	The ratio between two medium and light label partners.
Ratio M/L1	The ratio between two medium and light label partners.
Ratio M/L2	The ratio between two medium and light label partners.
Ratio M/L3	The ratio between two medium and light label partners.
Ratio M/L normalized	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized1	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized2	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized3	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L unmod. pep.	
Ratio M/L localized	
Ratio M/L nmods	
Ratio M/L variability [%]	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio M/L count	Number of redundant peptides (MS1 features) used for quantitation.
Ratio M/L iso-count	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio M/L type	
Ratio H/L	The ratio between two heavy and light label partners.
Ratio H/L1	The ratio between two heavy and light label partners.
Ratio H/L2	The ratio between two heavy and light label partners.
Ratio H/L3	The ratio between two heavy and light label partners.
Ratio H/L normalized	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized1	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized2	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized3	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L unmod. pep.	
Ratio H/L localized	
Ratio H/L nmods	
Ratio H/L variability [%]	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/L type	
Ratio H/L count	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/L iso-count	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/M	The ratio between two heavy and medium label partners.
Ratio H/M1	The ratio between two heavy and medium label partners.
Ratio H/M2	The ratio between two heavy and medium label partners.
Ratio H/M3	The ratio between two heavy and medium label partners.
Ratio H/M normalized	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized1	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized2	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized3	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M unmod. pep.	
Ratio H/M localized	
Ratio H/M nmods	

Ratio H/M variability [%]	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/M count	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/M iso-count	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/M type	
Occupancy L	
Occupancy M	
Occupancy H	
Ratio M/L C1	The ratio between two medium and light label partners.
Ratio M/L C11	The ratio between two medium and light label partners.
Ratio M/L C12	The ratio between two medium and light label partners.
Ratio M/L C13	The ratio between two medium and light label partners.
Ratio M/L normalized C1	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized C11	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized C12	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized C13	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L unmod. pep. C1	
Ratio M/L localized C1	
Ratio M/L nmods C1	
Ratio M/L variability [%] C1	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio M/L count C1	Number of redundant peptides (MS1 features) used for quantitation.
Ratio M/L iso-count C1	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio M/L type C1	
Ratio H/L C1	The ratio between two heavy and light label partners.
Ratio H/L C11	The ratio between two heavy and light label partners.
Ratio H/L C12	The ratio between two heavy and light label partners.
Ratio H/L C13	The ratio between two heavy and light label partners.
Ratio H/L normalized C1	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized C11	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized C12	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized C13	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L unmod. pep. C1	
Ratio H/L localized C1	
Ratio H/L nmods C1	
Ratio H/L variability [%] C1	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/L count C1	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/L iso-count C1	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/L type C1	
Ratio H/M C1	The ratio between two heavy and medium label partners.
Ratio H/M C11	The ratio between two heavy and medium label partners.
Ratio H/M C12	The ratio between two heavy and medium label partners.
Ratio H/M C13	The ratio between two heavy and medium label partners.
Ratio H/M normalized C1	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized C11	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized C12	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized C13	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.

Ratio H/M unmod. pep. C1	
Ratio H/M localized C1	
Ratio H/M nmods C1	
Ratio H/M variability [%] C1	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the
Ratio H/M count C1	naturally logarithmized ratios times 100. Number of redundant peptides (MS1 features) used for
Ratio H/M iso-count C1	quantitation. Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/M type C1	
Occupancy L C1	
Occupancy M C1	
Occupancy H C1	
Ratio M/L C2	The ratio between two medium and light label partners.
Ratio M/L C21	The ratio between two medium and light label partners.
Ratio M/L C22	The ratio between two medium and light label partners.
Ratio M/L C2 3	The ratio between two medium and light label partners.
Ratio M/L normalized C2	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized C21	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized C22	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized C23	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L unmod. pep. C2	
Ratio M/L localized C2	
Ratio M/L nmods C2	
Ratio M/L variability [%] C2	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio M/L count C2	Number of redundant peptides (MS1 features) used for quantitation.
Ratio M/L iso-count C2	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio M/L type C2	
Ratio H/L C2	The ratio between two heavy and light label partners.
Ratio H/L C21	The ratio between two heavy and light label partners.
Ratio H/L C22	The ratio between two heavy and light label partners.
Ratio H/L C23	The ratio between two heavy and light label partners.
Ratio H/L normalized C2	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized C21 Ratio H/L normalized C22	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1. Normalized ratio between two medium and light label partners.
Ratio H/L normalized C22 Ratio H/L normalized C2 3	The median of the total ratio population was shifted to 1. Normalized ratio between two medium and light label partners.
Ratio H/L unmod. pep. C2	The median of the total ratio population was shifted to 1.
Ratio H/L localized C2	
Ratio H/L nmods C2	
Ratio H/L variability [%] C2	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the
Ratio H/L count C2	naturally logarithmized ratios times 100. Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/L iso-count C2	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/L type C2	
Ratio H/M C2	The ratio between two heavy and medium label partners.
Ratio H/M C21	The ratio between two heavy and medium label partners.
Ratio H/M C22	The ratio between two heavy and medium label partners.
Ratio H/M C23	The ratio between two heavy and medium label partners.
Ratio H/M normalized C2	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized C21	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.

Ratio H/M normalized C22	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized C23	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M unmod. pep. C2	
Ratio H/M localized C2	
Ratio H/M nmods C2	
Ratio H/M variability [%] C2	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/M count C2	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/M iso-count C2	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/M type C2	
Occupancy L C2	
Occupancy M C2	
Occupancy H C2	
Ratio M/L C3	The ratio between two medium and light label partners.
Ratio M/L C3 1	The ratio between two medium and light label partners.
Ratio M/L C3 2	The ratio between two medium and light label partners.
Ratio M/L C3 3	The ratio between two medium and light label partners.
Ratio M/L normalized C3	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized C31	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized C32	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized C33	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L unmod. pep. C3	·
Ratio M/L localized C3	
Ratio M/L nmods C3	
Ratio M/L variability [%] C3	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio M/L count C3	Number of redundant peptides (MS1 features) used for quantitation.
Ratio M/L iso-count C3	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio M/L type C3	
Ratio H/L C3	The ratio between two heavy and light label partners.
Ratio H/L C31	The ratio between two heavy and light label partners.
Ratio H/L C32	The ratio between two heavy and light label partners.
Ratio H/L C33	The ratio between two heavy and light label partners.
Ratio H/L normalized C3	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized C31	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized C32	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized C33	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L unmod. pep. C3	
Ratio H/L localized C3	
Ratio H/L nmods C3	
Ratio H/L variability [%] C3	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/L count C3	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/L iso-count C3	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/L type C3	
Ratio H/M C3	The ratio between two heavy and medium label partners.
Ratio H/M C31	The ratio between two heavy and medium label partners.
Ratio H/M C32	The ratio between two heavy and medium label partners.

Ratio H/M normalized C3	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to
	1.
Ratio H/M normalized C31	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized C32	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized C33	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M unmod. pep. C3	
Ratio H/M localized C3	
Ratio H/M nmods C3	
Ratio H/M variability [%] C3	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/M count C3	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/M iso-count C3	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/M type C3	
Occupancy L C3	
Occupancy M C3	
Occupancy H C3	
Ratio M/L N1	The ratio between two medium and light label partners.
Ratio M/L N11	The ratio between two medium and light label partners.
Ratio M/L N12	The ratio between two medium and light label partners.
Ratio M/L N13	The ratio between two medium and light label partners.
Ratio M/L normalized N1	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized N11	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized N12	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized N13	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L unmod. pep. N1	
Ratio M/L localized N1	
Ratio M/L nmods N1	
Ratio M/L variability [%] N1	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio M/L count N1	Number of redundant peptides (MS1 features) used for quantitation.
Ratio M/L iso-count N1	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio M/L type N1	
Ratio H/L N1	The ratio between two heavy and light label partners.
Ratio H/L N11	The ratio between two heavy and light label partners.
Ratio H/L N12	The ratio between two heavy and light label partners.
Ratio H/L N13	The ratio between two heavy and light label partners.
Ratio H/L normalized N1	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized N11	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized N12	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized N13	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L unmod. pep. N1	
Ratio H/L localized N1	
Ratio H/L nmods N1	
Ratio H/L variability [%] N1	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/L count N1	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/L iso-count N1	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/L type N1	
Ratio H/M N1	The ratio between two heavy and medium label partners.

Ratio H/M N11	The ratio between two heavy and medium label partners.
Ratio H/M N12	The ratio between two heavy and medium label partners.
Ratio H/M N13	The ratio between two heavy and medium label partners.
Ratio H/M normalized N1	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized N11	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to
Ratio H/M normalized N12	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized N13	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M unmod. pep. N1	
Ratio H/M localized N1	
Ratio H/M nmods N1	
Ratio H/M variability [%] N1	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/M count N1	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/M iso-count N1	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/M type N1	
Occupancy L N1	
Occupancy M N1	
Occupancy H N1	
Ratio M/L N2	The ratio between two medium and light label partners.
Ratio M/L N21	The ratio between two medium and light label partners.
Ratio M/L N22	The ratio between two medium and light label partners.
Ratio M/L N23	The ratio between two medium and light label partners.
Ratio M/L normalized N2	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized N21	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized N22	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized N23	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L unmod. pep. N2	
Ratio M/L localized N2	
Ratio M/L nmods N2	
Ratio M/L variability [%] N2	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio M/L count N2	Number of redundant peptides (MS1 features) used for quantitation.
Ratio M/L iso-count N2	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio M/L type N2	
Ratio H/L N2	The ratio between two heavy and light label partners.
Ratio H/L N21	The ratio between two heavy and light label partners.
Ratio H/L N22	The ratio between two heavy and light label partners.
Ratio H/L N23	The ratio between two heavy and light label partners.
Ratio H/L normalized N2	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized N21	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized N22	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized N23	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L unmod. pep. N2	
Ratio H/L localized N2	
Ratio H/L nmods N2	
Ratio H/L variability [%] N2	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/L count N2	Number of redundant peptides (MS1 features) used for quantitation.
	- · ·

Ratio H/L iso-count N2	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/L type N2	
Ratio H/M N2	The ratio between two heavy and medium label partners.
Ratio H/M N2 1	The ratio between two heavy and medium label partners.
Ratio H/M N2 2	The ratio between two heavy and medium label partners.
Ratio H/M N2 3	The ratio between two heavy and medium label partners.
Ratio H/M normalized N2	
Ratio H/M normalized Nz	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized N21	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized N22	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized N23	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M unmod. pep. N2	
Ratio H/M localized N2	
Ratio H/M nmods N2	
Ratio H/M variability [%] N2	Coefficient of variability over all redundant quantifiable
	peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/M count N2	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/M iso-count N2	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/M type N2	
Occupancy L N2	
Occupancy M N2	
Occupancy H N2	
Ratio M/L N3	The ratio between two medium and light label partners.
Ratio M/L N31	The ratio between two medium and light label partners.
Ratio M/L N32	The ratio between two medium and light label partners.
Ratio M/L N3 3	The ratio between two medium and light label partners.
Ratio M/L normalized N3	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized N31	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized N32	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized N33	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L unmod. pep. N3	
Ratio M/L localized N3	
Ratio M/L nmods N3	
Ratio M/L variability [%] N3	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio M/L count N3	Number of redundant peptides (MS1 features) used for quantitation.
Ratio M/L iso-count N3	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio M/L type N3	
Ratio H/L N3	The ratio between two heavy and light label partners.
Ratio H/L N31	The ratio between two heavy and light label partners.
Ratio H/L N32	The ratio between two heavy and light label partners.
Ratio H/L N33	The ratio between two heavy and light label partners.
Ratio H/L normalized N3	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized N31	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized N32	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized N33	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L unmod. pep. N3	
Ratio H/L localized N3	

Ratio H/L variability [%] N3	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/L count N3	Number of redundant peptides (MS1 features) used for guantitation.
Ratio H/L iso-count N3	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/L type N3	
Ratio H/M N3	The ratio between two heavy and medium label partners.
Ratio H/M N3 1	The ratio between two heavy and medium label partners.
Ratio H/M N3 2	The ratio between two heavy and medium label partners.
Ratio H/M N3 3	The ratio between two heavy and medium label partners.
Ratio H/M normalized N3	Normalized ratio between two heavy and medium label
Ratio 17/W Hormalized NS	partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized N31	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized N32	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized N33	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M unmod. pep. N3	
Ratio H/M localized N3	
Ratio H/M nmods N3	
Ratio H/M variability [%] N3	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/M count N3	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/M iso-count N3	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/M type N3	
Occupancy L N3	
Occupancy M N3	
Occupancy H N3	
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 L	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the light label partner.
Intensity M	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the medium label partner.
Intensity H	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the heavy label partner.
Ratio mod/base L	
Ratio mod/base M	
Ratio mod/base H	
Intensity C1	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 L C1	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the light label partner.
Intensity M C1	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the medium label partner.
Intensity H C1	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the heavy label partner.
Ratio mod/base L C1	
Ratio mod/base M C1	
Ratio mod/base H C1	
Intensity C2	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 L C2	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the light label partner.
Intensity M C2	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the medium label partner.
Intensity H C2	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the heavy label partner.
Ratio mod/base L C2	

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Ratio mod/base M C2	
Ratio mod/base H C2	
Intensity C3	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 L C3	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the light label partner.
Intensity M C3	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the medium label partner.
Intensity H C3	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the heavy label partner.
Ratio mod/base L C3	
Ratio mod/base M C3	
Ratio mod/base H C3	
Intensity N1	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 L N1	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the light label partner.
Intensity M N1	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the medium label partner.
Intensity H N1	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the heavy label partner.
Ratio mod/base L N1	
Ratio mod/base M N1	
Ratio mod/base H N1	
Intensity N2	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 L N2	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the light label partner.
Intensity M N2	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the medium label partner.
Intensity H N2	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the heavy label partner.
Ratio mod/base L N2	
Ratio mod/base M N2	
Ratio mod/base H N2	
Intensity N3	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 L N3	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the light label partner.
Intensity M N3	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the medium label partner.
Intensity H N3	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the heavy label partner.
Ratio mod/base L N3	
Ratio mod/base M N3	
Ratio mod/base H N3	
Occupancy C1	
Occupancy ratioC1	
Occupancy error scale C1	
Occupancy C2	
Occupancy ratioC2	
Occupancy error scale C2	
Occupancy C3	
Occupancy ratioC3	
Occupancy error scale C3	
Occupancy N1	
Occupancy ratioN1	
Occupancy error scale N1	
Occupancy N2	
ia	
Occupancy ratioN2	
Occupancy ratioN2 Occupancy error scale N2	
' '	
Occupancy error scale N2	

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
Potential contaminant	analysis. 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	

SUMO3Sites

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 psoition 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.
Protein names		Names of proteins this peptide is associated with.
Gene names		Names of genes 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 C1		
Score diff C1		
PEP C1		
Score C1		
Localization prob C2		
Score diff C2		
PEP C2		
Score C2		
Localization prob C3		
Score diff C3		
PEP C3		
Score C3		
Localization prob N1		
Score diff N1		
PEP N1		
Score N1		
Localization prob N2		
Score diff N2		
PEP N2		
Score N2		
Localization prob N3		
Score diff N3		
PEP N3		
Score N3		
Diagnostic peak		
Number of SUMO3		Different numbers of SUMO3 on peptides that this site is involved in.
Amino acid		
Sequence window		
Modification window		
Peptide window coverage		
SUMO3 Probabilities		
SUMO3 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 C1		Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type C2		Indicates whether this experiment was identified by MS/MS or only by matching between runs.

Identification type C3	Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type N1	Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type N2	Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type N3	Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Ratio M/L	The ratio between two medium and light label partners.
Ratio M/L1	The ratio between two medium and light label partners.
Ratio M/L2	The ratio between two medium and light label partners.
Ratio M/L3	The ratio between two medium and light label partners.
Ratio M/L normalized	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized1	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized2	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized3	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L unmod. pep.	
Ratio M/L localized	
Ratio M/L nmods	
Ratio M/L variability [%]	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio M/L count	Number of redundant peptides (MS1 features) used for quantitation.
Ratio M/L iso-count	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio M/L type	
Ratio H/L	The ratio between two heavy and light label partners.
Ratio H/L1	The ratio between two heavy and light label partners.
Ratio H/L2	The ratio between two heavy and light label partners.
Ratio H/L3	The ratio between two heavy and light label partners.
Ratio H/L normalized	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized1	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized2	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized3	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L unmod. pep.	
Ratio H/L localized	
Ratio H/L nmods	
Ratio H/L variability [%]	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/L type	
Ratio H/L count	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/L iso-count	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/M	The ratio between two heavy and medium label partners.
Ratio H/M1	The ratio between two heavy and medium label partners.
Ratio H/M2	The ratio between two heavy and medium label partners.
Ratio H/M3	The ratio between two heavy and medium label partners.
Ratio H/M normalized	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized1	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized2	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized3	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M unmod. pep.	
Ratio H/M localized	
Ratio H/M nmods	

Ratio H/M variability [%]	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/M count	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/M iso-count	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/M type	
Occupancy L	
Occupancy M	
Occupancy H	
Ratio M/L C1	The ratio between two medium and light label partners.
Ratio M/L C11	The ratio between two medium and light label partners.
Ratio M/L C12	The ratio between two medium and light label partners.
Ratio M/L C13	The ratio between two medium and light label partners.
Ratio M/L normalized C1	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized C11	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized C12	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized C13	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L unmod. pep. C1	
Ratio M/L localized C1	
Ratio M/L nmods C1	
Ratio M/L variability [%] C1	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio M/L count C1	Number of redundant peptides (MS1 features) used for quantitation.
Ratio M/L iso-count C1	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio M/L type C1	
Ratio H/L C1	The ratio between two heavy and light label partners.
Ratio H/L C11	The ratio between two heavy and light label partners.
Ratio H/L C12	The ratio between two heavy and light label partners.
Ratio H/L C13	The ratio between two heavy and light label partners.
Ratio H/L normalized C1	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized C11	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized C12	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized C13	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L unmod. pep. C1	
Ratio H/L localized C1	
Ratio H/L nmods C1	
Ratio H/L variability [%] C1	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/L count C1	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/L iso-count C1	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/L type C1	
Ratio H/M C1	The ratio between two heavy and medium label partners.
Ratio H/M C11	The ratio between two heavy and medium label partners.
Ratio H/M C12	The ratio between two heavy and medium label partners.
Ratio H/M C13	The ratio between two heavy and medium label partners.
Ratio H/M normalized C1	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized C11	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized C12	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized C13	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.

Ratio H/M unmod. pep. C1	
Ratio H/M localized C1	
Ratio H/M nmods C1	
Ratio H/M variability [%] C1	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the
Ratio H/M count C1	naturally logarithmized ratios times 100. Number of redundant peptides (MS1 features) used for
Ratio H/M iso-count C1	quantitation. Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/M type C1	
Occupancy L C1	
Occupancy M C1	
Occupancy H C1	
Ratio M/L C2	The ratio between two medium and light label partners.
Ratio M/L C21	The ratio between two medium and light label partners.
Ratio M/L C22	The ratio between two medium and light label partners.
Ratio M/L C2 3	The ratio between two medium and light label partners.
Ratio M/L normalized C2	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized C21	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized C22	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized C23	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L unmod. pep. C2	
Ratio M/L localized C2	
Ratio M/L nmods C2	
Ratio M/L variability [%] C2	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio M/L count C2	Number of redundant peptides (MS1 features) used for quantitation.
Ratio M/L iso-count C2	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio M/L type C2	
Ratio H/L C2	The ratio between two heavy and light label partners.
Ratio H/L C21	The ratio between two heavy and light label partners.
Ratio H/L C22	The ratio between two heavy and light label partners.
Ratio H/L C23	The ratio between two heavy and light label partners.
Ratio H/L normalized C2	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized C21 Ratio H/L normalized C22	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1. Normalized ratio between two medium and light label partners.
Ratio H/L normalized C22 Ratio H/L normalized C2 3	The median of the total ratio population was shifted to 1. Normalized ratio between two medium and light label partners.
Ratio H/L unmod. pep. C2	The median of the total ratio population was shifted to 1.
Ratio H/L localized C2	
Ratio H/L nmods C2	
Ratio H/L variability [%] C2	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the
Ratio H/L count C2	naturally logarithmized ratios times 100. Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/L iso-count C2	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/L type C2	
Ratio H/M C2	The ratio between two heavy and medium label partners.
Ratio H/M C21	The ratio between two heavy and medium label partners.
Ratio H/M C22	The ratio between two heavy and medium label partners.
Ratio H/M C23	The ratio between two heavy and medium label partners.
Ratio H/M normalized C2	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized C21	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.

Ratio H/M normalized C22	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized C23	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M unmod. pep. C2	
Ratio H/M localized C2	
Ratio H/M nmods C2	
Ratio H/M variability [%] C2	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/M count C2	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/M iso-count C2	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/M type C2	
Occupancy L C2	
Occupancy M C2	
Occupancy H C2	
Ratio M/L C3	The ratio between two medium and light label partners.
Ratio M/L C3 1	The ratio between two medium and light label partners.
Ratio M/L C3 2	The ratio between two medium and light label partners.
Ratio M/L C3 3	The ratio between two medium and light label partners.
Ratio M/L normalized C3	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized C31	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized C32	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized C33	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L unmod. pep. C3	·
Ratio M/L localized C3	
Ratio M/L nmods C3	
Ratio M/L variability [%] C3	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio M/L count C3	Number of redundant peptides (MS1 features) used for quantitation.
Ratio M/L iso-count C3	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio M/L type C3	
Ratio H/L C3	The ratio between two heavy and light label partners.
Ratio H/L C31	The ratio between two heavy and light label partners.
Ratio H/L C32	The ratio between two heavy and light label partners.
Ratio H/L C33	The ratio between two heavy and light label partners.
Ratio H/L normalized C3	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized C31	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized C32	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized C33	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L unmod. pep. C3	
Ratio H/L localized C3	
Ratio H/L nmods C3	
Ratio H/L variability [%] C3	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/L count C3	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/L iso-count C3	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/L type C3	
Ratio H/M C3	The ratio between two heavy and medium label partners.
Ratio H/M C31	The ratio between two heavy and medium label partners.
Ratio H/M C32	The ratio between two heavy and medium label partners.

Ratio H/M normalized C3	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to
	1.
Ratio H/M normalized C31	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized C32	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized C33	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M unmod. pep. C3	
Ratio H/M localized C3	
Ratio H/M nmods C3	
Ratio H/M variability [%] C3	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/M count C3	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/M iso-count C3	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/M type C3	
Occupancy L C3	
Occupancy M C3	
Occupancy H C3	
Ratio M/L N1	The ratio between two medium and light label partners.
Ratio M/L N11	The ratio between two medium and light label partners.
Ratio M/L N12	The ratio between two medium and light label partners.
Ratio M/L N13	The ratio between two medium and light label partners.
Ratio M/L normalized N1	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized N11	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized N12	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized N13	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L unmod. pep. N1	
Ratio M/L localized N1	
Ratio M/L nmods N1	
Ratio M/L variability [%] N1	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio M/L count N1	Number of redundant peptides (MS1 features) used for quantitation.
Ratio M/L iso-count N1	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio M/L type N1	
Ratio H/L N1	The ratio between two heavy and light label partners.
Ratio H/L N11	The ratio between two heavy and light label partners.
Ratio H/L N12	The ratio between two heavy and light label partners.
Ratio H/L N13	The ratio between two heavy and light label partners.
Ratio H/L normalized N1	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized N11	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized N12	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized N13	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L unmod. pep. N1	
Ratio H/L localized N1	
Ratio H/L nmods N1	
Ratio H/L variability [%] N1	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/L count N1	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/L iso-count N1	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/L type N1	
Ratio H/M N1	The ratio between two heavy and medium label partners.

Ratio H/M N11	The ratio between two heavy and medium label partners.
Ratio H/M N12	The ratio between two heavy and medium label partners.
Ratio H/M N13	The ratio between two heavy and medium label partners.
Ratio H/M normalized N1	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized N11	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to
Ratio H/M normalized N12	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized N13	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M unmod. pep. N1	
Ratio H/M localized N1	
Ratio H/M nmods N1	
Ratio H/M variability [%] N1	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/M count N1	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/M iso-count N1	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/M type N1	
Occupancy L N1	
Occupancy M N1	
Occupancy H N1	
Ratio M/L N2	The ratio between two medium and light label partners.
Ratio M/L N21	The ratio between two medium and light label partners.
Ratio M/L N22	The ratio between two medium and light label partners.
Ratio M/L N23	The ratio between two medium and light label partners.
Ratio M/L normalized N2	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized N21	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized N22	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized N23	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L unmod. pep. N2	
Ratio M/L localized N2	
Ratio M/L nmods N2	
Ratio M/L variability [%] N2	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio M/L count N2	Number of redundant peptides (MS1 features) used for quantitation.
Ratio M/L iso-count N2	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio M/L type N2	
Ratio H/L N2	The ratio between two heavy and light label partners.
Ratio H/L N21	The ratio between two heavy and light label partners.
Ratio H/L N22	The ratio between two heavy and light label partners.
Ratio H/L N23	The ratio between two heavy and light label partners.
Ratio H/L normalized N2	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized N21	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized N22	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized N23	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L unmod. pep. N2	
Ratio H/L localized N2	
Ratio H/L nmods N2	
Ratio H/L variability [%] N2	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/L count N2	Number of redundant peptides (MS1 features) used for quantitation.
	- · ·

Ratio H/L iso-count N2	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/L type N2	
Ratio H/M N2	The ratio between two heavy and medium label partners.
Ratio H/M N2 1	The ratio between two heavy and medium label partners.
Ratio H/M N2 2	The ratio between two heavy and medium label partners.
Ratio H/M N2 3	The ratio between two heavy and medium label partners.
Ratio H/M normalized N2	
Ratio H/M normalized Nz	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized N21	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized N22	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized N23	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M unmod. pep. N2	
Ratio H/M localized N2	
Ratio H/M nmods N2	
Ratio H/M variability [%] N2	Coefficient of variability over all redundant quantifiable
	peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/M count N2	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/M iso-count N2	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/M type N2	
Occupancy L N2	
Occupancy M N2	
Occupancy H N2	
Ratio M/L N3	The ratio between two medium and light label partners.
Ratio M/L N31	The ratio between two medium and light label partners.
Ratio M/L N32	The ratio between two medium and light label partners.
Ratio M/L N3 3	The ratio between two medium and light label partners.
Ratio M/L normalized N3	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized N31	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized N32	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L normalized N33	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L unmod. pep. N3	
Ratio M/L localized N3	
Ratio M/L nmods N3	
Ratio M/L variability [%] N3	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio M/L count N3	Number of redundant peptides (MS1 features) used for quantitation.
Ratio M/L iso-count N3	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio M/L type N3	
Ratio H/L N3	The ratio between two heavy and light label partners.
Ratio H/L N31	The ratio between two heavy and light label partners.
Ratio H/L N32	The ratio between two heavy and light label partners.
Ratio H/L N33	The ratio between two heavy and light label partners.
Ratio H/L normalized N3	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized N31	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized N32	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L normalized N33	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L unmod. pep. N3	
Ratio H/L localized N3	

Ratio H/L variability [%] N3	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/L count N3	Number of redundant peptides (MS1 features) used for guantitation.
Ratio H/L iso-count N3	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/L type N3	
Ratio H/M N3	The ratio between two heavy and medium label partners.
Ratio H/M N3 1	The ratio between two heavy and medium label partners.
Ratio H/M N3 2	The ratio between two heavy and medium label partners.
Ratio H/M N3 3	The ratio between two heavy and medium label partners.
Ratio H/M normalized N3	Normalized ratio between two heavy and medium label
Ratio 17/W Hormalized NS	partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized N31	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized N32	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M normalized N33	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M unmod. pep. N3	
Ratio H/M localized N3	
Ratio H/M nmods N3	
Ratio H/M variability [%] N3	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/M count N3	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/M iso-count N3	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/M type N3	
Occupancy L N3	
Occupancy M N3	
Occupancy H N3	
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 L	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the light label partner.
Intensity M	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the medium label partner.
Intensity H	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the heavy label partner.
Ratio mod/base L	
Ratio mod/base M	
Ratio mod/base H	
Intensity C1	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 L C1	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the light label partner.
Intensity M C1	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the medium label partner.
Intensity H C1	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the heavy label partner.
Ratio mod/base L C1	
Ratio mod/base M C1	
Ratio mod/base H C1	
Intensity C2	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 L C2	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the light label partner.
Intensity M C2	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the medium label partner.
Intensity H C2	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the heavy label partner.
Ratio mod/base L C2	

D.: 1/1 1100	
Ratio mod/base M C2	
Ratio mod/base H C2	
Intensity C3	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 L C3	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the light label partner.
Intensity M C3	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the medium label partner.
Intensity H C3	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the heavy label partner.
Ratio mod/base L C3	
Ratio mod/base M C3	
Ratio mod/base H C3	
Intensity N1	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 L N1	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the light label partner.
Intensity M N1	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the medium label partner.
Intensity H N1	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the heavy label partner.
Ratio mod/base L N1	
Ratio mod/base M N1	
Ratio mod/base H N1	
Intensity N2	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 L N2	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the light label partner.
Intensity M N2	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the medium label partner.
Intensity H N2	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the heavy label partner.
Ratio mod/base L N2	
Ratio mod/base M N2	
Ratio mod/base H N2	
Intensity N3	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 L N3	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the light label partner.
Intensity M N3	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the medium label partner.
Intensity H N3	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the heavy label partner.
Ratio mod/base L N3	
Ratio mod/base M N3	
Ratio mod/base H N3	
Occupancy C1	
Occupancy ratioC1	
Occupancy error scale C1	
Occupancy C2	
Occupancy ratioC2	
Occupancy error scale C2	
Occupancy C3	
Occupancy ratioC3	
Occupancy error scale C3	
Occupancy N1	
Occupancy ratioN1	
Occupancy error scale N1	
Occupancy N2	
ia	
Occupancy ratioN2	
Occupancy ratioN2 Occupancy error scale N2	
' '	
Occupancy error scale N2	

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
Potential contaminant	analysis. 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, occuring 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, occuring 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, occuring 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.
Protein names		Name(s) of protein(s) contained within the group.
Gene names		Name(s) of the gene(s) associated to the protein(s) contained within the group.
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 colum '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 C1		Number of peptides (distinct peptide sequences) in experiment C1
Peptides C2		Number of peptides (distinct peptide sequences) in experiment C2
Peptides C3		Number of peptides (distinct peptide sequences) in experiment C3
Peptides N1		Number of peptides (distinct peptide sequences) in experiment N1
Peptides N2		Number of peptides (distinct peptide sequences) in experiment N2
Peptides N3		Number of peptides (distinct peptide sequences) in experiment N3
Razor + unique peptides C1		Number of razor + unique peptides (distinct peptide sequences) in experiment C1
Razor + unique peptides C2		Number of razor + unique peptides (distinct peptide sequences) in experiment C2
Razor + unique peptides C3		Number of razor + unique peptides (distinct peptide sequences) in experiment C3
Razor + unique peptides N1		Number of razor + unique peptides (distinct peptide sequences) in experiment N1
Razor + unique peptides N2		Number of razor + unique peptides (distinct peptide sequences) in experiment N2
Razor + unique peptides N3		Number of razor + unique peptides (distinct peptide sequences) in experiment N3
Unique peptides C1		Number of unique peptides (distinct peptide sequences) in experiment C1
Unique peptides C2		Number of unique peptides (distinct peptide sequences) in experiment C2
Unique peptides C3		Number of unique peptides (distinct peptide sequences) in experiment C3
Unique peptides N1		Number of unique peptides (distinct peptide sequences) in experiment N1
Unique peptides N2		Number of unique peptides (distinct peptide sequences) in experiment N2

Unique peptides N3	Number of unique peptides (distinct peptide sequences) in experiment N3
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.
Identification type C1	Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type C2	Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type C3	Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type N1	Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type N2	Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Identification type N3	Indicates whether this experiment was identified by MS/MS or only by matching between runs.
Ratio M/L	The ratio between two medium and light label partners.
Ratio M/L normalized	Normalized ratio between two heavy and light label partners.
	The median of the total ratio population was shifted to 1.
Ratio M/L variability [%]	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio M/L count	Number of redundant peptides (MS1 features) used for quantitation.
Ratio M/L iso-count	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio M/L type	
Ratio H/L	The ratio between two heavy and light label partners.
Ratio H/L normalized	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L variability [%]	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/L count	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/L iso-count	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/L type	
Ratio H/M	The ratio between two heavy and medium label partners.
Ratio H/M normalized	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M variability [%]	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/M count	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/M iso-count	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/M type	
Ratio M/L C1	The ratio between two medium and light label partners.
Ratio M/L normalized C1	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L variability [%] C1	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio M/L count C1	Number of redundant peptides (MS1 features) used for quantitation.
Ratio M/L iso-count C1	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio M/L type C1	

Ratio H/L normalized C1	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L variability [%] C1	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/L count C1	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/L iso-count C1	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/L type C1	
Ratio H/M C1	The ratio between two heavy and medium label partners.
Ratio H/M normalized C1	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M variability [%] C1	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/M count C1	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/M iso-count C1	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/M type C1	
Ratio M/L C2	The ratio between two medium and light label partners.
Ratio M/L normalized C2	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L variability [%] C2	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio M/L count C2	Number of redundant peptides (MS1 features) used for quantitation.
Ratio M/L iso-count C2	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio M/L type C2	
Ratio H/L C2	The ratio between two heavy and light label partners.
Ratio H/L normalized C2	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L variability [%] C2	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/L count C2	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/L iso-count C2	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/L type C2	
Ratio H/M C2	The ratio between two heavy and medium label partners.
Ratio H/M normalized C2	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M variability [%] C2	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/M count C2	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/M iso-count C2	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/M type C2	
Ratio M/L C3	The ratio between two medium and light label partners.
Ratio M/L normalized C3	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L variability [%] C3	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio M/L count C3	Number of redundant peptides (MS1 features) used for quantitation.
Ratio M/L iso-count C3	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio M/L type C3	
Ratio H/L C3	The ratio between two heavy and light label partners.
Ratio H/L normalized C3	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L variability [%] C3	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/L count C3	Number of redundant peptides (MS1 features) used for quantitation.

Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
The state of the s
The ratio between two heavy and medium label partners.
Normalized ratio between two heavy and medium label
partners. The median of the total ratio population was shifted to 1.
Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Number of redundant peptides (MS1 features) used for quantitation.
Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
The ratio between two medium and light label partners.
Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Number of redundant peptides (MS1 features) used for quantitation.
Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
The ratio between two heavy and light label partners.
Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Number of redundant peptides (MS1 features) used for quantitation.
Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
The ratio between two heavy and medium label partners.
Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Number of redundant peptides (MS1 features) used for quantitation.
Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
The ratio between two medium and light label partners.
Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Number of redundant peptides (MS1 features) used for quantitation.
Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
The ratio between two heavy and light label partners.
Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Number of redundant peptides (MS1 features) used for quantitation.
Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
The ratio between two heavy and medium label partners.
Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.

Ratio H/M variability [%] N2	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the
Ratio H/M count N2	naturally logarithmized ratios times 100. Number of redundant peptides (MS1 features) used for
Ratio H/M iso-count N2	quantitation. Number of redundant peptides (MS1 features) used for
5	quantitation that are quantified with the re-quantify method.
Ratio H/M type N2	The vetic heating on true and diversional limits labely a cuttorial
Ratio M/L N3 Ratio M/L normalized N3	The ratio between two medium and light label partners.
	Normalized ratio between two heavy and light label partners. The median of the total ratio population was shifted to 1.
Ratio M/L variability [%] N3	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio M/L count N3	Number of redundant peptides (MS1 features) used for quantitation.
Ratio M/L iso-count N3	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio M/L type N3	
Ratio H/L N3	The ratio between two heavy and light label partners.
Ratio H/L normalized N3	Normalized ratio between two medium and light label partners. The median of the total ratio population was shifted to 1.
Ratio H/L variability [%] N3	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/L count N3	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/L iso-count N3	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/L type N3	
Ratio H/M N3	The ratio between two heavy and medium label partners.
Ratio H/M normalized N3	Normalized ratio between two heavy and medium label partners. The median of the total ratio population was shifted to 1.
Ratio H/M variability [%] N3	Coefficient of variability over all redundant quantifiable peptides. It is calculated as the standard deviation of the naturally logarithmized ratios times 100.
Ratio H/M count N3	Number of redundant peptides (MS1 features) used for quantitation.
Ratio H/M iso-count N3	Number of redundant peptides (MS1 features) used for quantitation that are quantified with the re-quantify method.
Ratio H/M type N3	
Sequence coverage C1 [%]	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 C2 [%]	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 C3 [%]	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 N1 [%]	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 N2 [%]	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 N3 [%]	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 L	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the light label partner.
Intensity M	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the medium label partner.
Intensity H	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the heavy label partner.
Intensity C1	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 L C1	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the light label partner.
Intensity M C1	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the medium label partner.
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Intensity H C1	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the heavy label partner.
Intensity C2	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 L C2	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the light label partner.
Intensity M C2	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the medium label partner.
Intensity H C2	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the heavy label partner.
Intensity C3	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 L C3	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the light label partner.
Intensity M C3	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the medium label partner.
Intensity H C3	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the heavy label partner.
Intensity N1	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 L N1	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the light label partner.
Intensity M N1	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the medium label partner.
Intensity H N1	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the heavy label partner.
Intensity N2	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 L N2	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the light label partner.
Intensity M N2	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the medium label partner.
Intensity H N2	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the heavy label partner.
Intensity N3	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 L N3	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the light label partner.
Intensity M N3	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the medium label partner.
Intensity H N3	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the heavy label partner.
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
DOCUMO/INIO	identifying the peptides of this protein, referenced against the msms table.
Deamidation (NQ) site IDs	Identifier(s) for site(s) associated with the protein group, which show(s) evidence of the modification, referenced against the appropriate modification site file.

Oxidation (M) site IDs	Identifier(s) for site(s) associated with the protein group, which show(s) evidence of the modification, referenced against the appropriate modification site file.
Phospho (S) 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.
SUMO3 site IDs	Identifier(s) for site(s) associated with the protein group, which show(s) evidence of the modification, referenced against the appropriate modification site file.
Deamidation (NQ) site positions	Positions of the sites in the leading protein of this group.
Oxidation (M) site positions	Positions of the sites in the leading protein of this group.
Phospho (S) site positions	Positions of the sites in the leading protein of this group.
SUMO3 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.
Туре		The type of detection for the peptide. SILAC – A SILAC pair 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 – 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.
Max intensity m/z 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.
Max intensity m/z 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.
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.
Lys Count	The number of instances of Lys contained within the sequence. The value for this can reliably be determined in the case of SILAC partners, based on the distance between the partners. These counts are used to solidify the peptide identification process.
Arg Count	The number of instances of Arg contained within the sequence. The value for this can reliably be determined in the case of SILAC partners, based on the distance between the partners. These counts are used to solidify the peptide identification process.
Ratio M/L	The ratio between two medium and light multiplet members.
Ratio M/L normalized	Normalized ratio between two medium and light multiplet members. The median of the total ratio population was shifted to 1.
Ratio H/L	The ratio between two heavy and light multiplet members.
Ratio H/L normalized	Normalized ratio between two heavy and light multiplet members. The median of the total ratio population was shifted to 1.
Ratio H/M	The ratio between two heavy and medium multiplet members.
Ratio H/M normalized	Normalized ratio between two heavy and medium multiplet members. The median of the total ratio population was shifted to 1.
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 L	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the light label partner.
Intensity M	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the medium label partner.
Intensity H	Summed up eXtracted Ion Current (XIC) of the isotopic cluster linked to the heavy label partner.
Intensities L	The intensity values of the light SILAC partner isotopes.
Intensities M	The intensity values of the medium SILAC partner isotopes.
Intensities H	The intensity values of the heavy SILAC partner 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 SILAC States	The SILAC partner detected for the peptide. The value 0 is always the light partner. In the case of double SILAC labeling 1 is the heavy partner. In the case of triple SILAC labeling 1 is the medium and 2 the heavy partner.
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 of second chromatography.
Multiplets / s		The average number of labeling multiplets detected per of second 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.
Туре		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 he 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 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.
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

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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.	Mass analyzer		FTMS – Fourier transform ICR or orbitrap cell.
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.	Туре		isotopic cluster. PEAK – single peak.
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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.	Mass Error [ppm]		
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PEP Posterior Error Probability of the identification. This value essentially operates as a p-value, where smaller is more significant.	Retention time		
	PEP		Posterior Error Probability of the identification. This value essentially operates as a p-value, where smaller is more
Poolo I Induidinga aggic for the deal gaaggared wich/la specific	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.
Labeling State	Labeling state of the precursor isotope pattern used to identify the peptide.
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 he MS spectrum.
Precursor Full ScanNumber	The full scannumber 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 SUMO3 K	
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'.
Deamidation (NQ) site IDs	Identifier of the oxidation summary stored in the file 'Deamidation (NQ)Sites.txt'.
Oxidation (M) site IDs	Identifier of the oxidation summary stored in the file 'Oxidation (M)Sites.txt'.
Phospho (S) site IDs	Identifier of the oxidation summary stored in the file 'Phospho (S)Sites.txt'.
SUMO3 site IDs	Identifier of the oxidation summary stored in the file 'SUMO3Sites.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.
Deamidation (NQ) site IDs		
Oxidation (M) site IDs		
Phospho (S) site IDs		
SUMO3 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.
Deamidation (NQ) Probabilities		
Oxidation (M) Probabilities		
Phospho (S) Probabilities		
SUMO3 Probabilities		
Deamidation (NQ) Score Diffs		
Oxidation (M) Score Diffs		
Phospho (S) Score Diffs		
SUMO3 Score Diffs		
Acetyl (Protein N-term)		
Deamidation (NQ)		
Oxidation (M)		
Phospho (S)		
SUMO3 Proteins		The IPI identifiers of the proteins the identified peptide is
Chargo		associated with.
Charge		The charge of the precursor ion.
Mass		The mass-over-charge of the precursor ion. 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.