Report for PEP Section in mzTab File

example_7

The PEP section of the mzTab file contains 5,729 quantified peptide features measured in 2 samples.

	number of peptides	
quantified	5,729	100%
quantified (any zero)	230	4.01%
quantified (any NaN)	503	8.78%
identified (total)	5,729	100%
identified (unique modified)	5,102	89.06%
identified (unique stripped)	4,826	84.24%

Table 1: Total number of quantified and identified peptides. (any zero) corresponds to peptides which are absent in one or more samples. (any NaN) corresponds to peptides which could not be quantified due to overlapping peptide features.

mod	specificity	number
Dimethyl	N-term	4037
Dimethyl	K	2482
Dimethyl:2H(4)13C(2)	N-term	1692
Dimethyl:2H(4)13C(2)	K	1168
Carbamidomethyl	C	679

Table 2: Statistics of modifications.

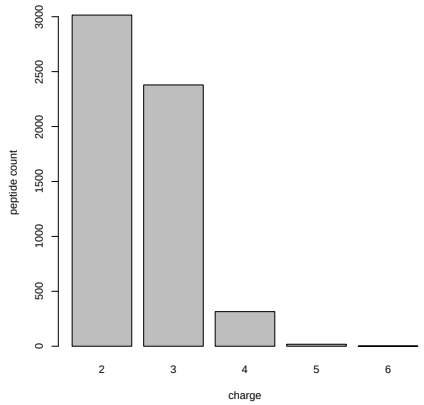


Figure 1: Charge distribution of peptide quantifications.

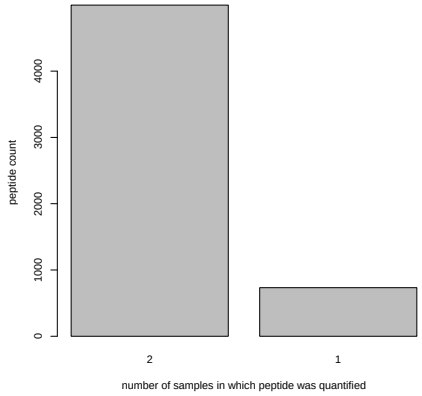


Figure 2: Frequency plot of peptide quantifications.

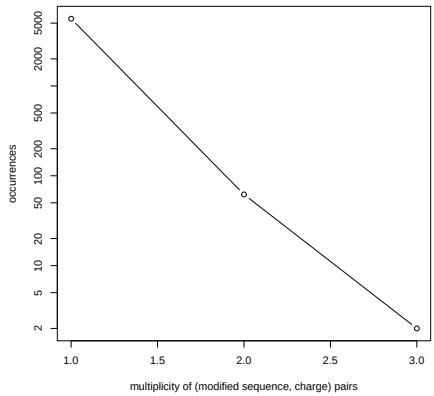


Figure 3: (modified sequence, charge) pair multiplicity vs frequency plot. Each peptide feature (characterised by a (possibly) modified peptide sequence and a charge state) should ideally occur only once in the analysis. In other words, peptides of multiplicity 1 should have a very high frequency. The plot below should show a significant spike on the left and can be used as QC of the analysis.

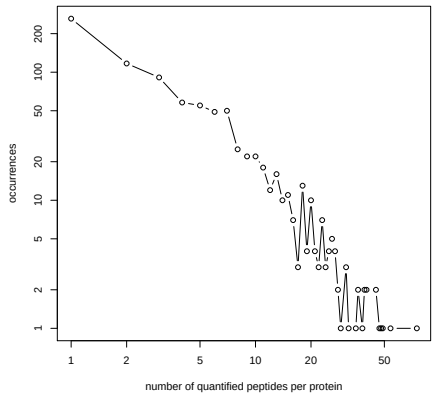


Figure 4: Number of quantified peptides per protein.

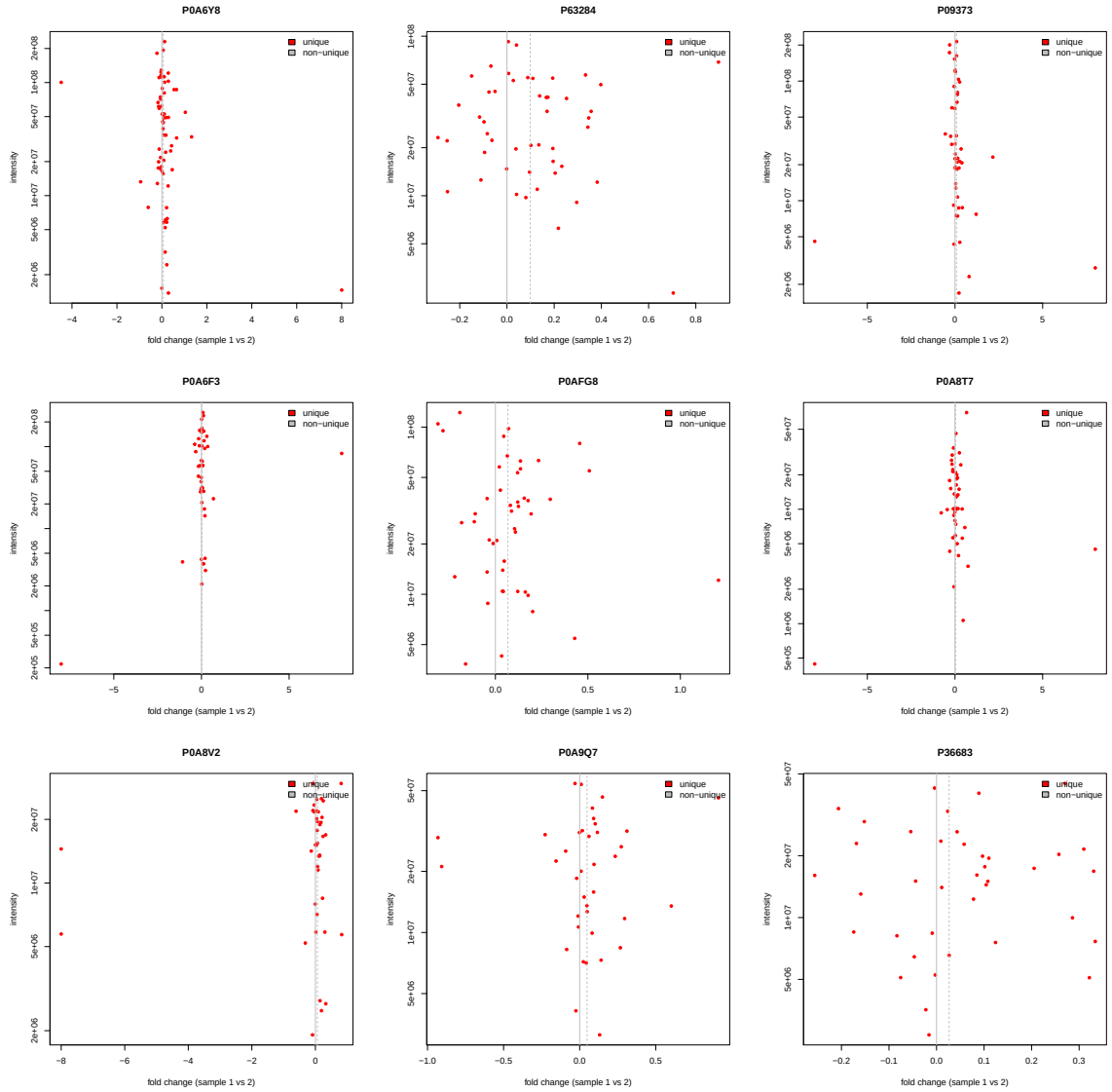
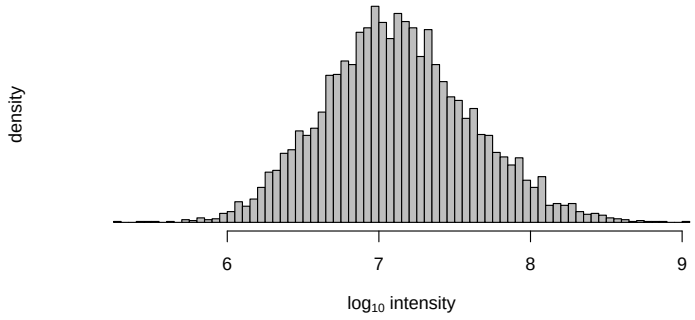
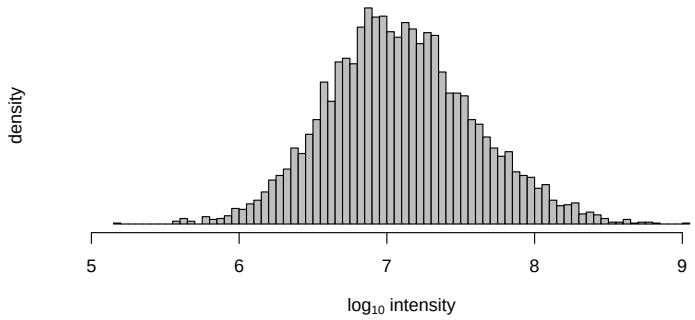


Figure 5: Fold changes of peptide abundances 1 and 2. For proteins with the largest number of quantified peptides.



(a) peptide abundances 1, median(intensity) = $12,328,450$



(b) peptide abundances 2, median(intensity) = $11,432,500$

Figure 6: peptide abundance distributions.

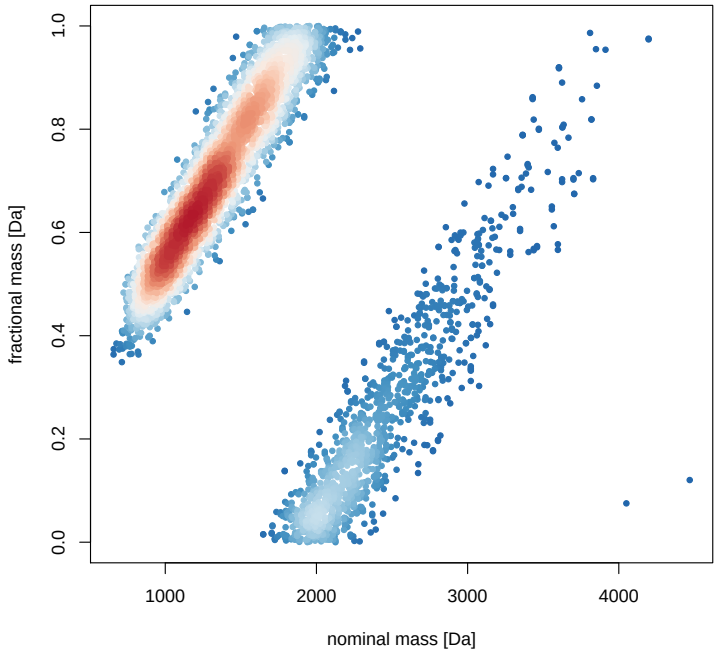


Figure 7: Kendrick nominal fractional mass plot

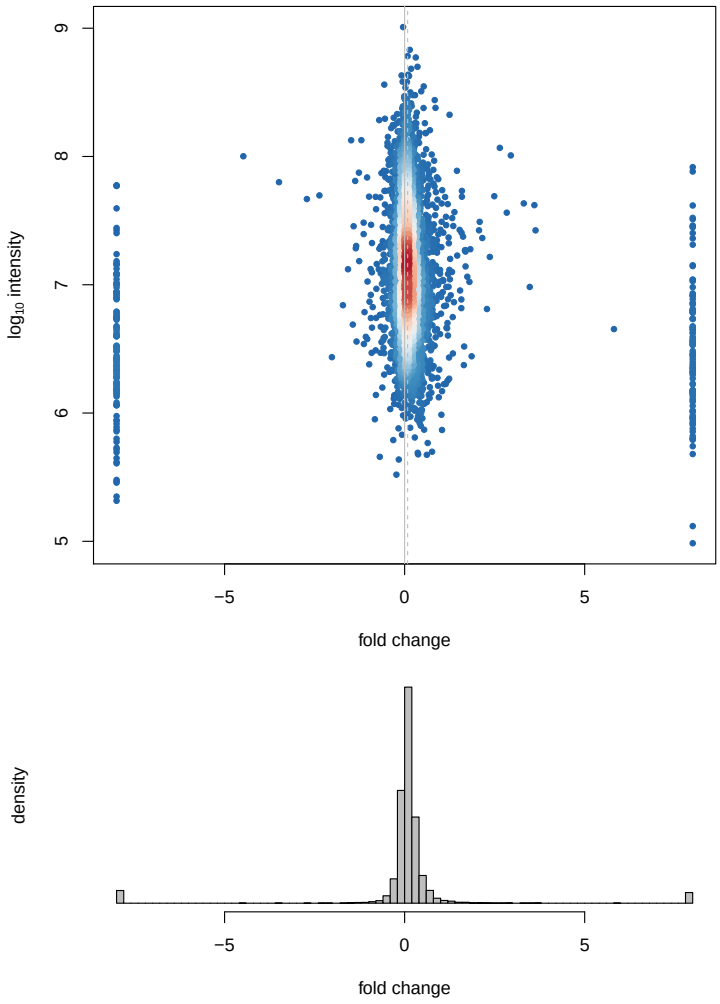


Figure 8: Fold changes of peptide abundances 1 and 2.
median(fc) = 0.0838 sd(fc) = 1.7142

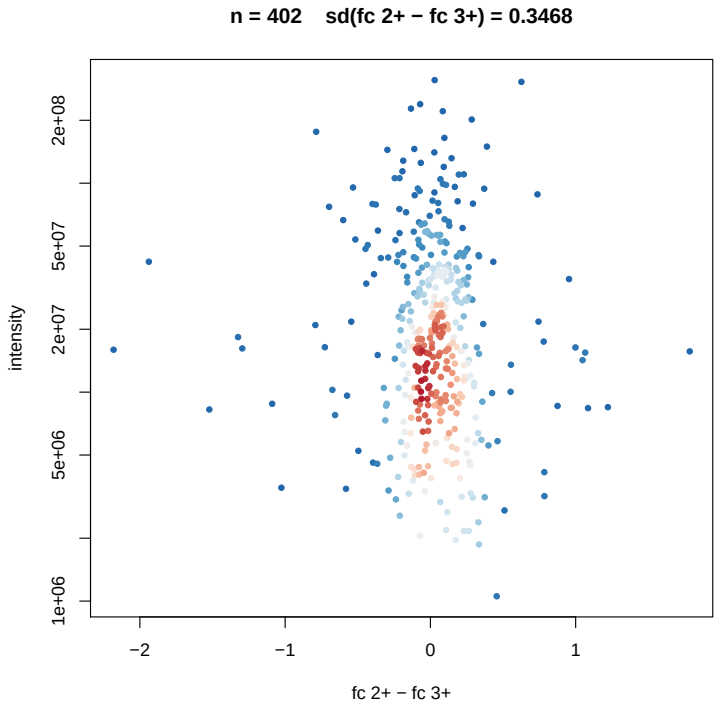


Figure 9: Fold changes of the same peptide in charge 2+ and 3+ are expected to be identical. Here we plot the difference of the 2+ and 3+ fold changes of sample 1 vs. sample 2 of all peptides which were identified and quantified in both charge states.

modified sequence	accession	charge	retention time	m/z
no matching sequences found				

Table 3: Peptides of interest. Please note that the script requires a vector of *stripped* peptides sequences, but in the above table we list the *modified* peptide sequences.

modified sequence	accession	charge	retention time	m/z
	no matching accessions found			

Table 4: Proteins of interest.