

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%
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.

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.

sample	finite	zero	nan
1	5315	125	289
2	5410	105	214

Table 3: Statistics of quantifications.

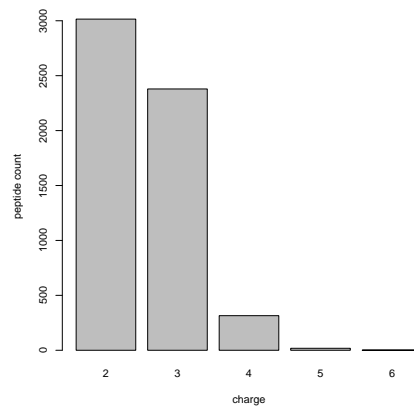


Figure 1: Charge distribution of peptide quantifications.

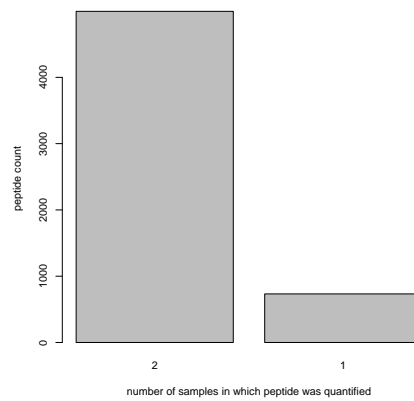


Figure 2: Frequency plot of peptide quantifications.

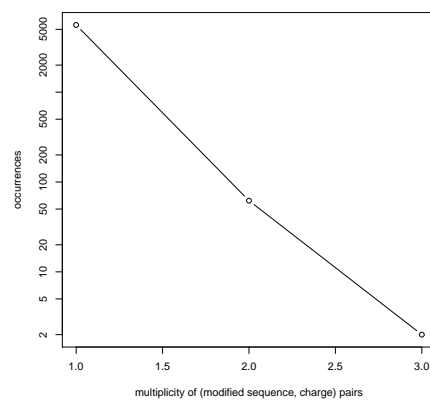


Figure 3: (modified sequence, charge) pair multiplicity vs frequency plot. Each peptide feature (characterised by a (possibly) modified peptide sequence and a charge state) should ideally occur only once in the analysis. In other words, peptides of multiplicity 1 should have a very high frequency. The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

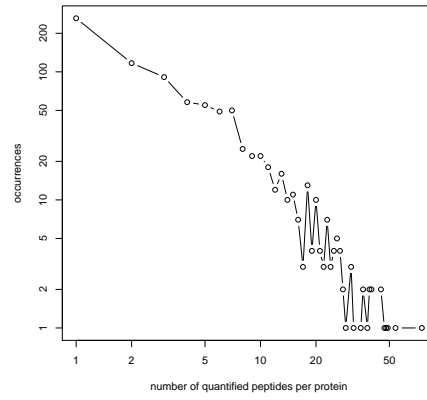


Figure 4: Number of quantified peptides per protein.

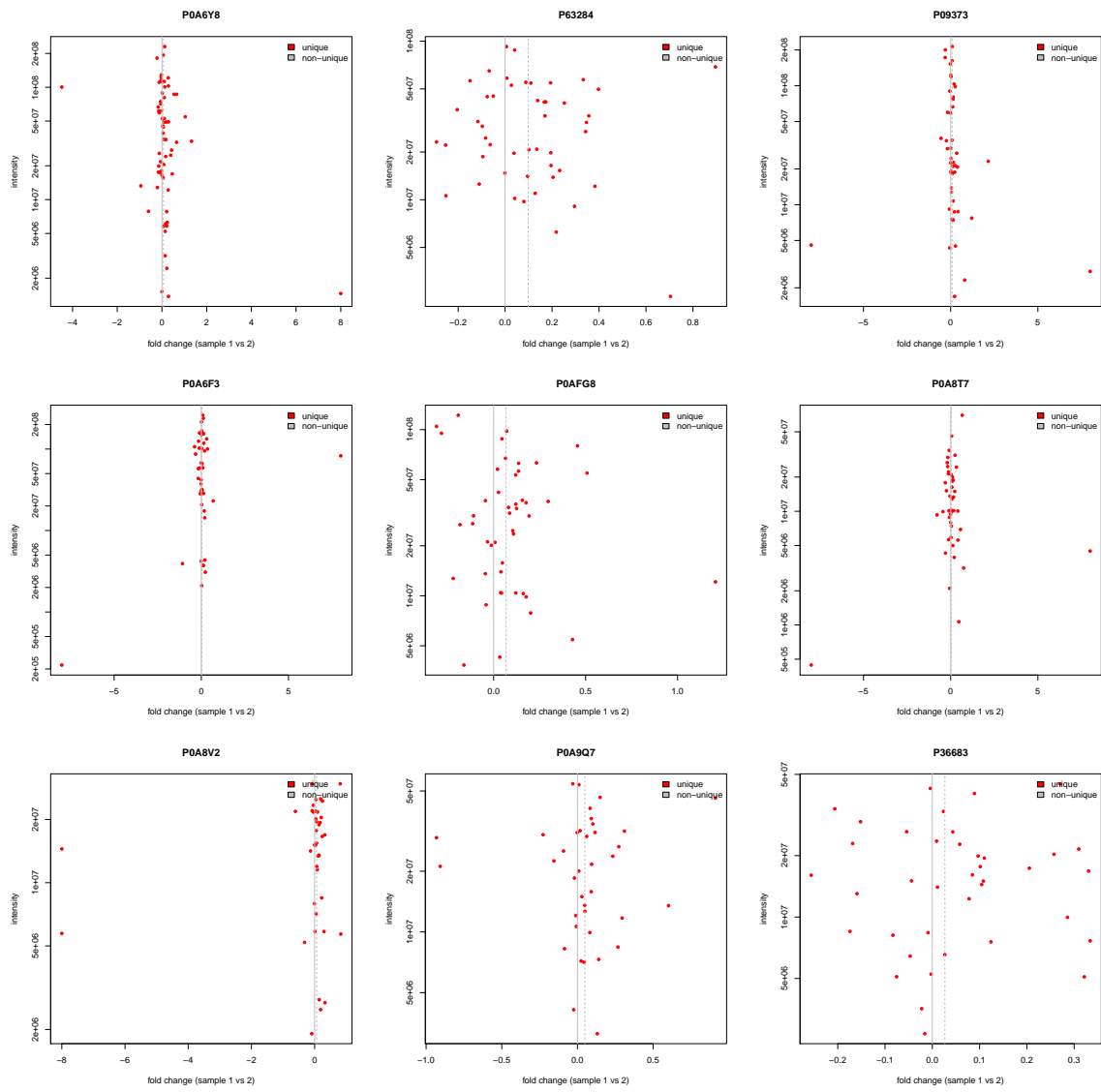
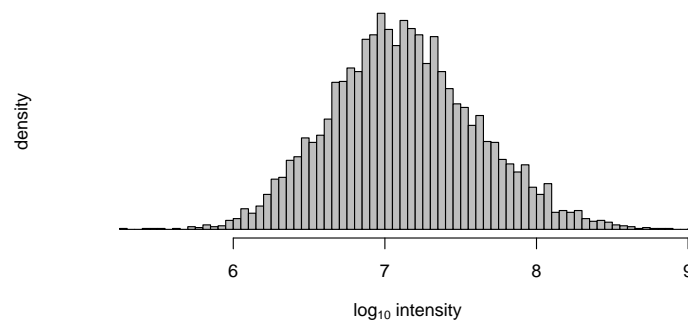
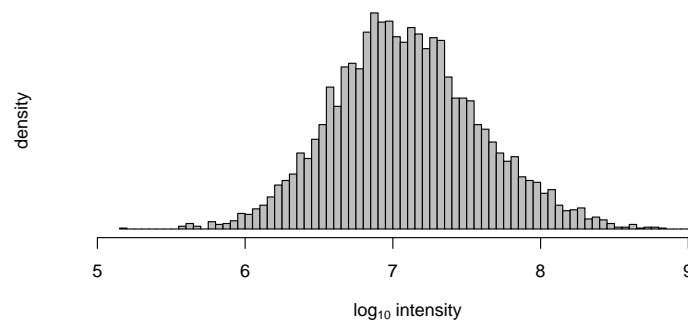


Figure 5: Fold changes of peptide abundances 1 and 2. For proteins with the largest number of quantified peptides.



(a) peptide abundances 1, $\text{median}(\text{intensity}) = 12,328,450$



(b) peptide abundances 2, $\text{median}(\text{intensity}) = 11,432,500$

Figure 6: peptide abundance distributions.

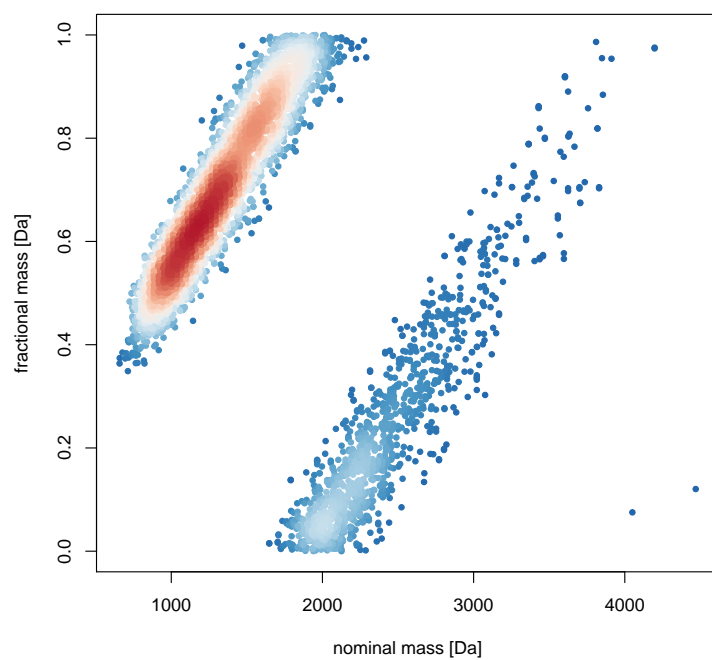


Figure 7: Kendrick nominal fractional mass plot

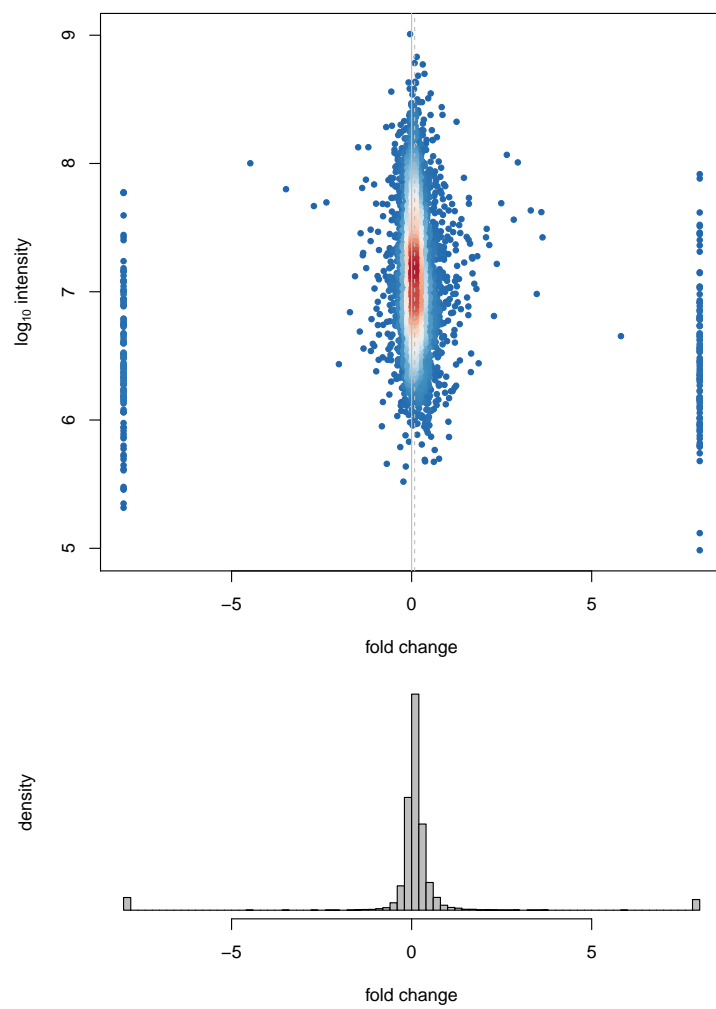


Figure 8: Fold changes of peptide abundances 1 and 2.
 $\text{median}(\text{fc}) = 0.0838$ $\text{sd}(\text{fc}) = 1.7142$

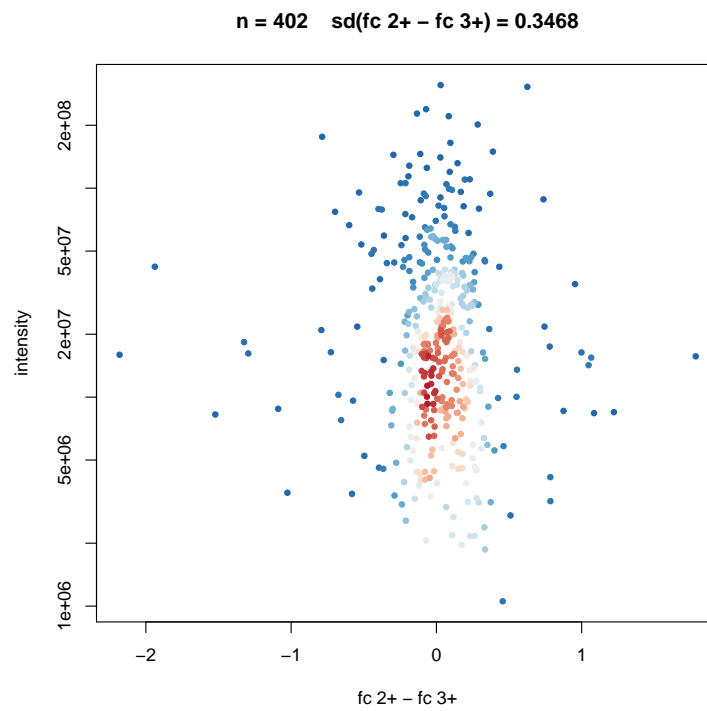


Figure 9: Fold changes of the same peptide in charge 2+ and 3+ are expected to be identical. Here we plot the difference of the 2+ and 3+ fold changes of sample 1 vs. sample 2 of all peptides which were identified and quantified in both charge states.

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

Table 4: 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 5: Proteins of interest.