

## Report for PEP Section in mzTab File example\_2

The PEP section of the **mzTab** file contains 2,160 quantified peptide features measured in 2 samples.

	number of peptides	
quantified	2,160	100%
identified (total)	2,160	100%
identified (unique modified)	2,021	93.56%
identified (unique stripped)	1,926	89.17%

Table 1: Total number of quantified and identified peptides.

mod	specificity	number
Carbamidomethyl	C	205

Table 2: Statistics of modifications.

sample	finite	zero	nan
1	2160	0	0
2	2160	0	0

Table 3: Statistics of quantifications.

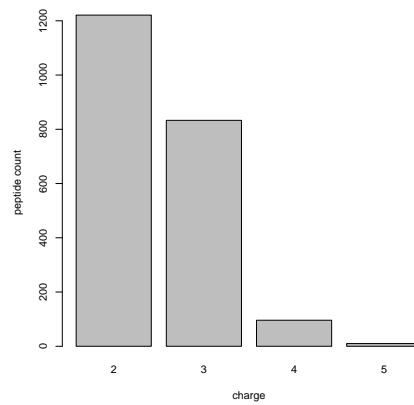


Figure 1: Charge distribution of peptide quantifications.

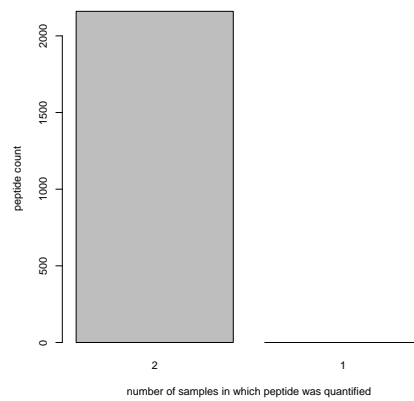


Figure 2: Frequency plot of peptide quantifications.

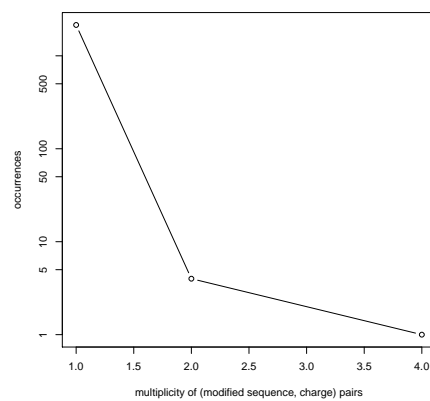


Figure 3: (modified sequence, charge) pair multiplicity vs frequency plot. Each peptide feature (characterised by a (possibly) modified peptide sequence and a charge state) should ideally occur only once in the analysis. In other words, peptides of multiplicity 1 should have a very high frequency. The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

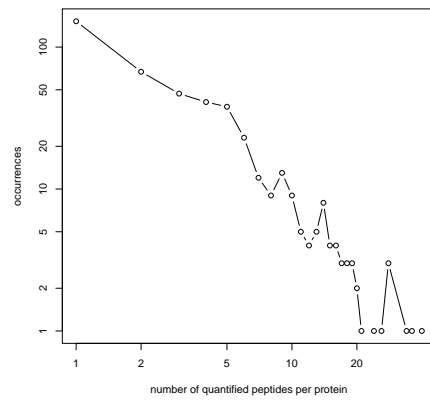


Figure 4: Number of quantified peptides per protein.

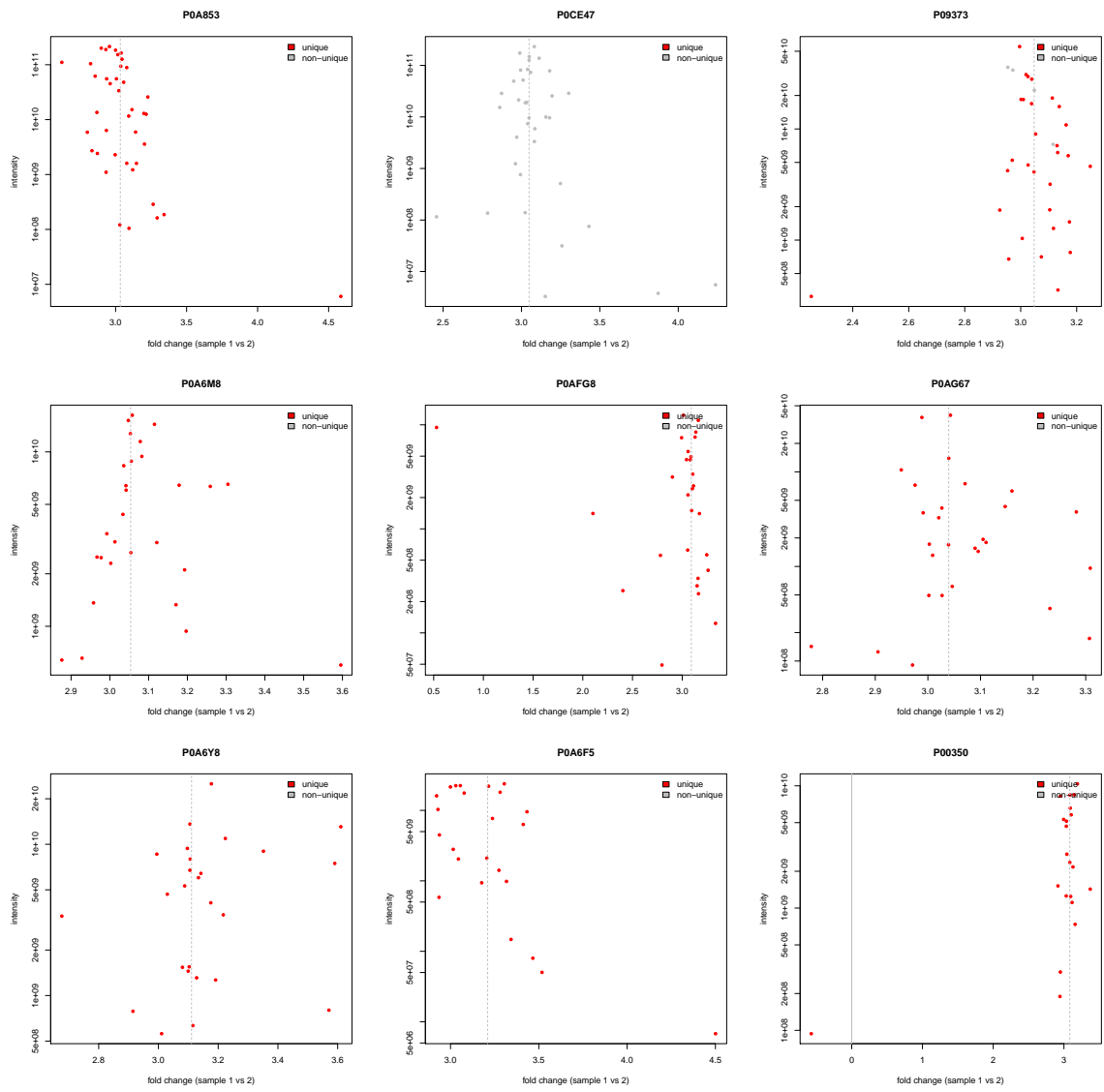
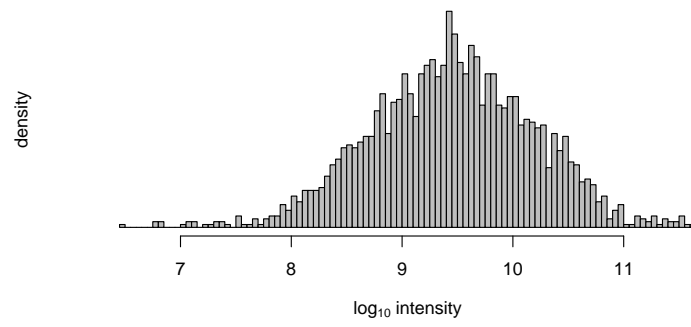
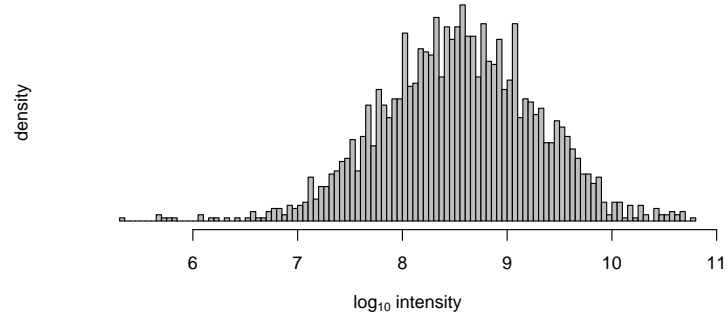


Figure 5: Fold changes of peptide abundances 1 and 2. For proteins with the largest number of quantified peptides.



(a) peptide abundances 1,  $\text{median}(\text{intensity}) = 2,858,004,992$



(b) peptide abundances 2,  $\text{median}(\text{intensity}) = 348,081,008$

Figure 6: peptide abundance distributions.

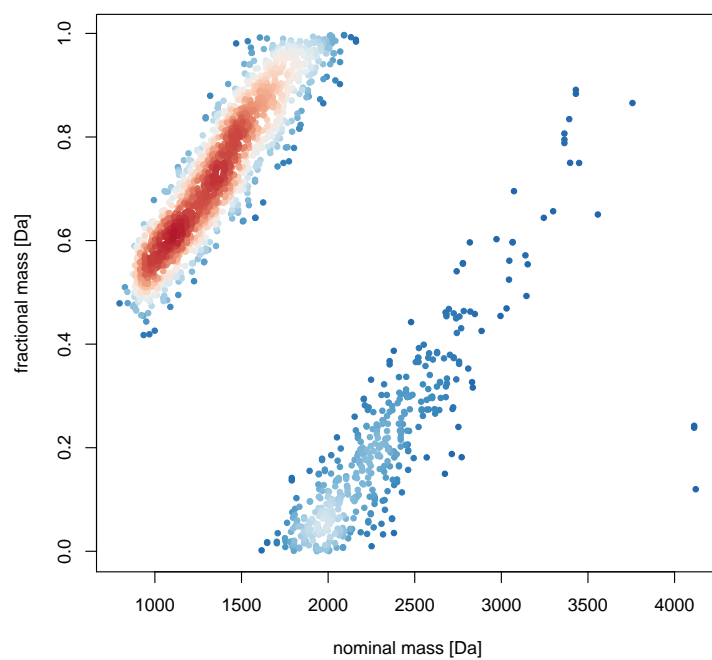


Figure 7: Kendrick nominal fractional mass plot

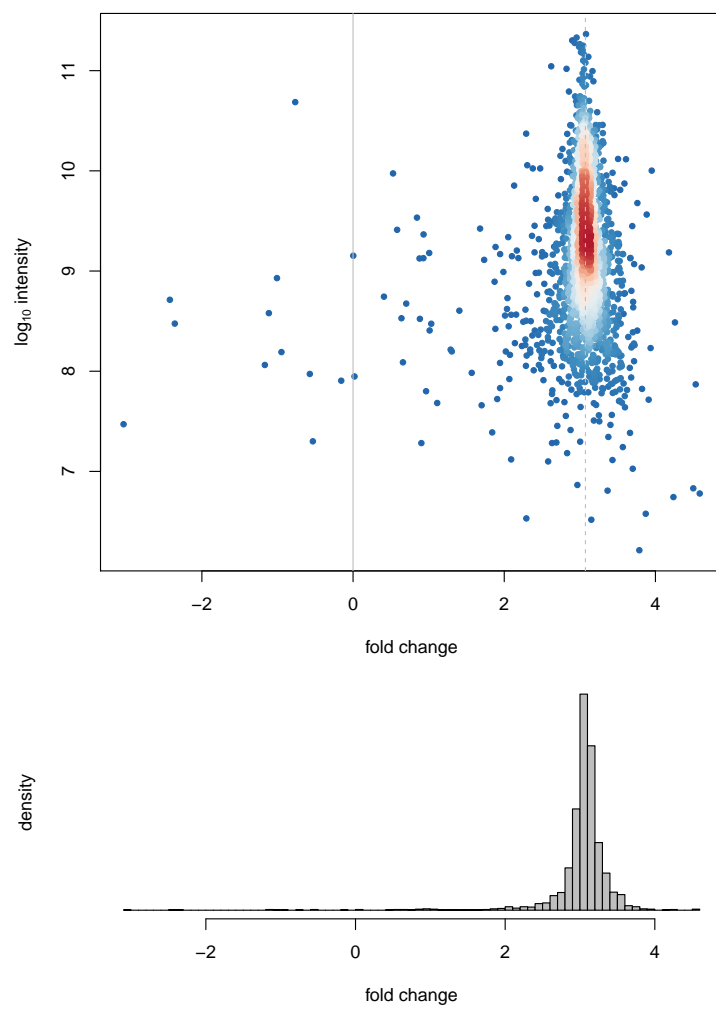


Figure 8: Fold changes of peptide abundances 1 and 2.  
 $\text{median}(\text{fc}) = 3.0739$      $\text{sd}(\text{fc}) = 0.4645$

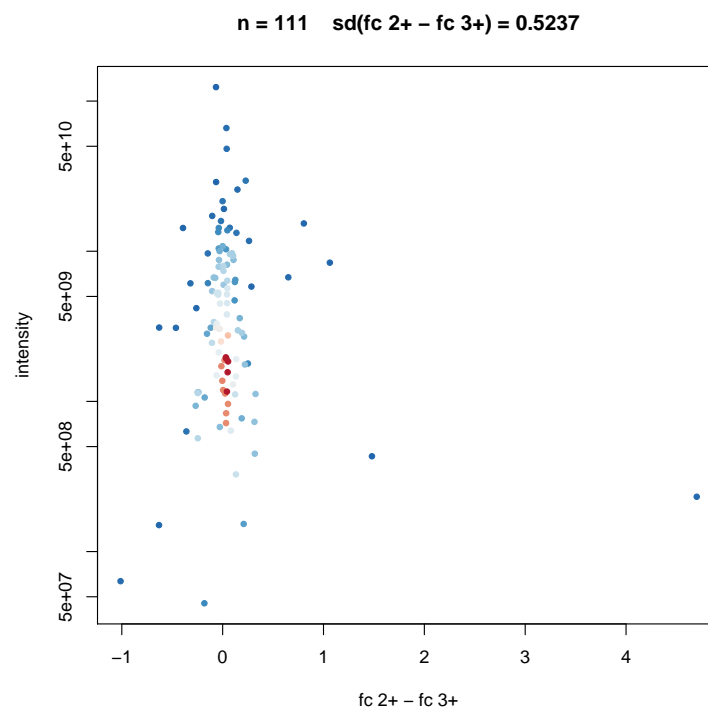


Figure 9: Fold changes of the same peptide in charge 2+ and 3+ are expected to be identical. Here we plot the difference of the 2+ and 3+ fold changes of sample 1 vs. sample 2 of all peptides which were identified and quantified in both charge states.

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.