

# Report for PEP Section in mzTab File

## example\_5

The PEP section of the **mzTab** file contains 45,072 quantified peptide features measured in 54 samples.

	number of peptides
quantified	45,072
identified (total)	45,072
identified (unique modified)	35,080
identified (unique stripped)	31,307

Table 1: Total number of quantified and identified peptides.

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

Table 2: Peptides of interest. 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 3: Proteins of interest.

mod	specificity	number
Oxidation	M	8798
Methylthio	C	7927
Dioxidation	M	372
Label:13C(6)15N(4)	R	89
Label:13C(6)15N(2)	K	79

Table 4: Statistics of modifications.

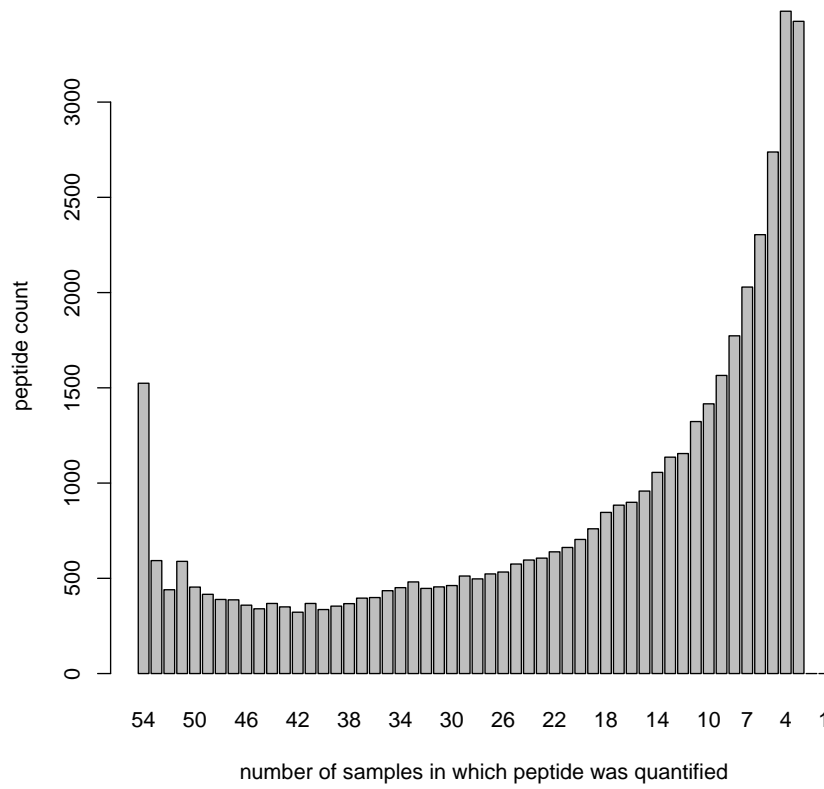


Figure 1: Frequency plot of peptide quantifications.

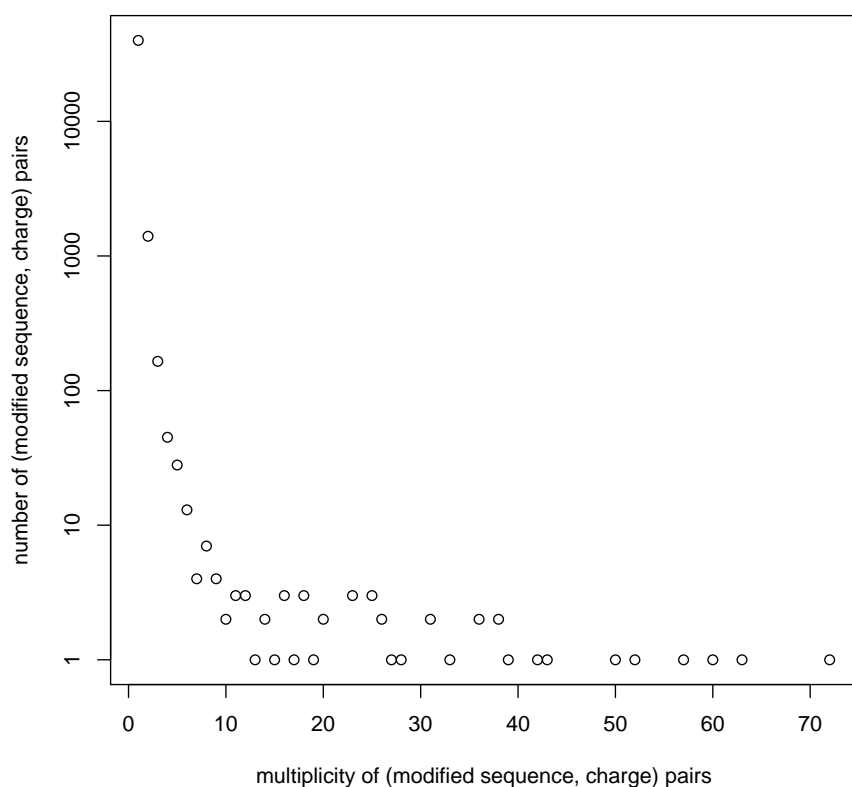
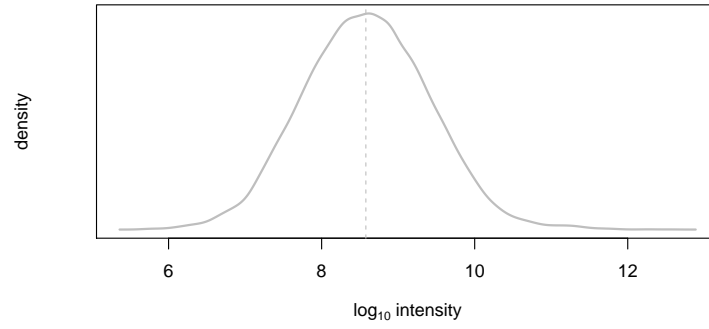
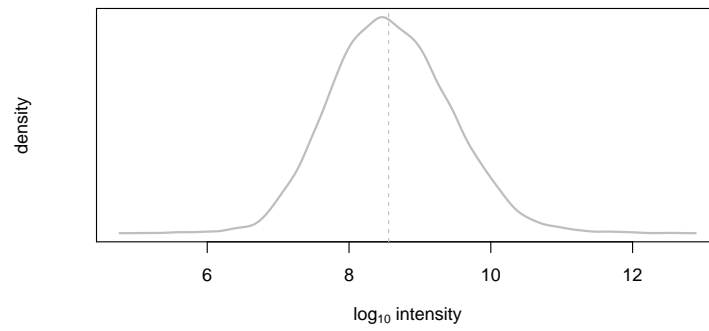


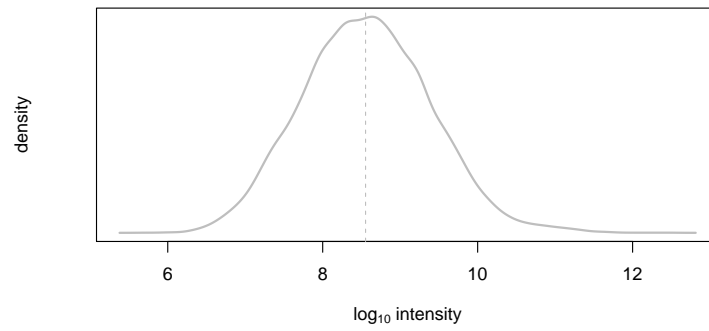
Figure 2: (modified sequence, charge) pair multiplicity vs frequency plot. Each peptide feature (characterised by a (possibly) modified peptide sequence and a charge state) should ideally occur only once in the analysis. In other words, peptides of multiplicity 1 should have a very high frequency. The plot below should show a significant spike on the left and can be used as QC of the analysis.



(a) peptide abundances 1,  $\text{median}(\text{intensity}) = 378,509,488$



(b) peptide abundances 2,  $\text{median}(\text{intensity}) = 362,260,000$



(c) peptide abundances 3,  $\text{median}(\text{intensity}) = 357,520,000$

Figure 3: peptide abundance distributions.

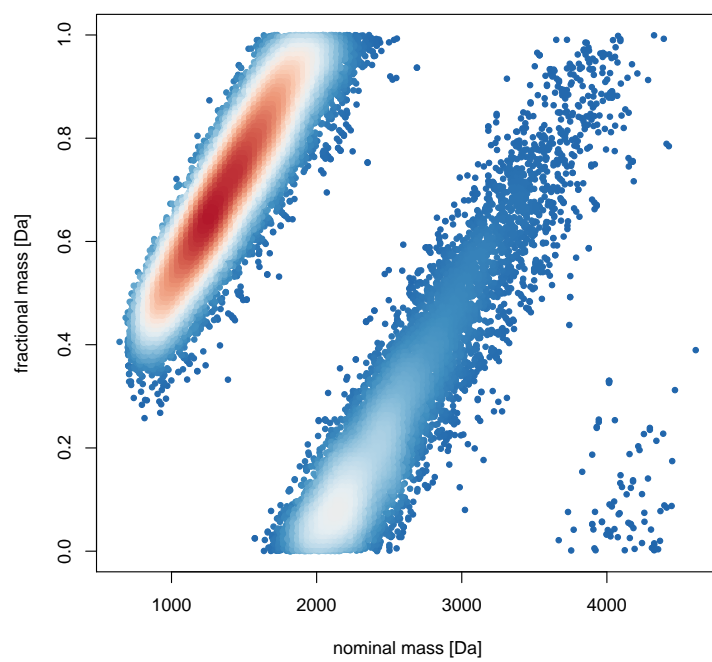


Figure 4: Kendrick nominal fractional mass plot

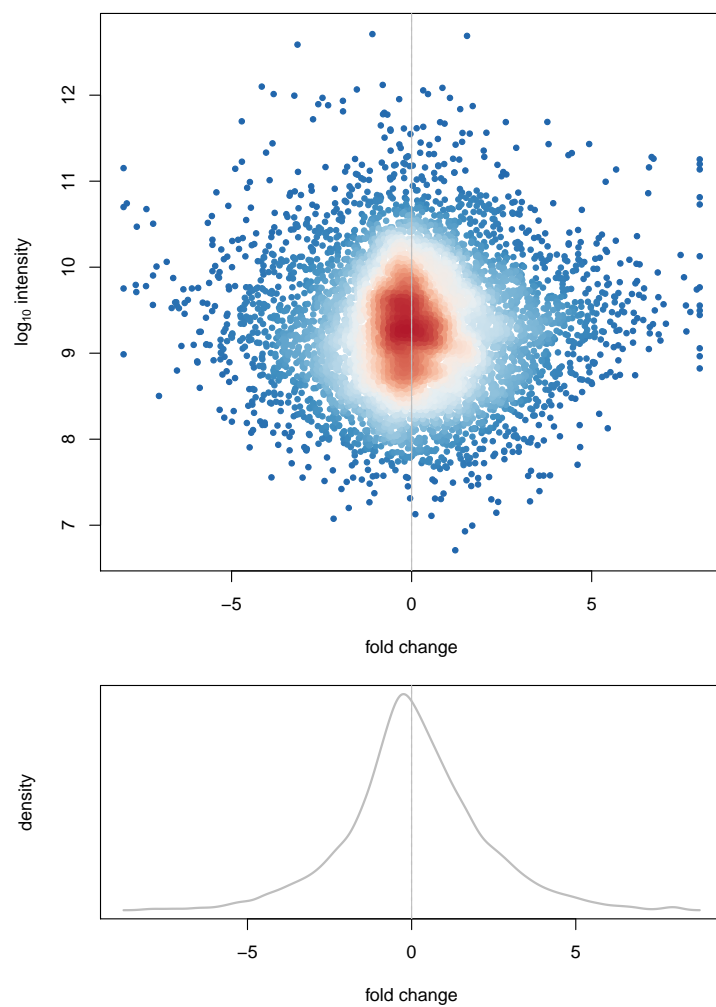


Figure 5: Fold changes of peptide abundances 1 and 2.  
 $\text{median}(\text{fc}) = -0.0034$        $\text{sd}(\text{fc}) = 2.0759$

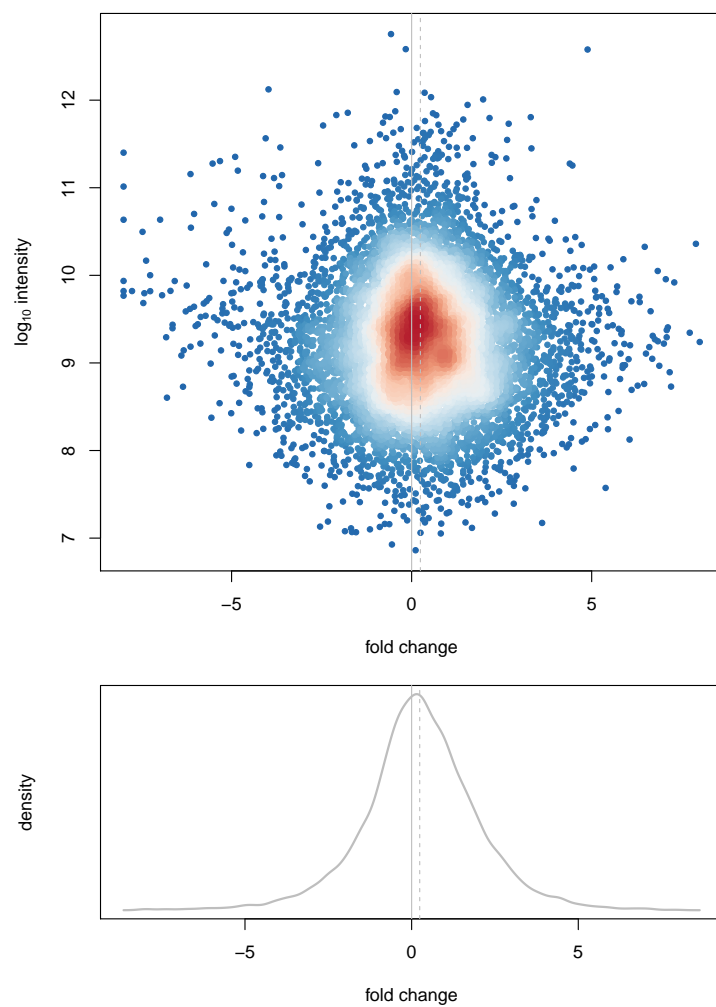


Figure 6: Fold changes of peptide abundances 1 and 3.  
 $\text{median}(\text{fc}) = 0.2428$        $\text{sd}(\text{fc}) = 1.7662$

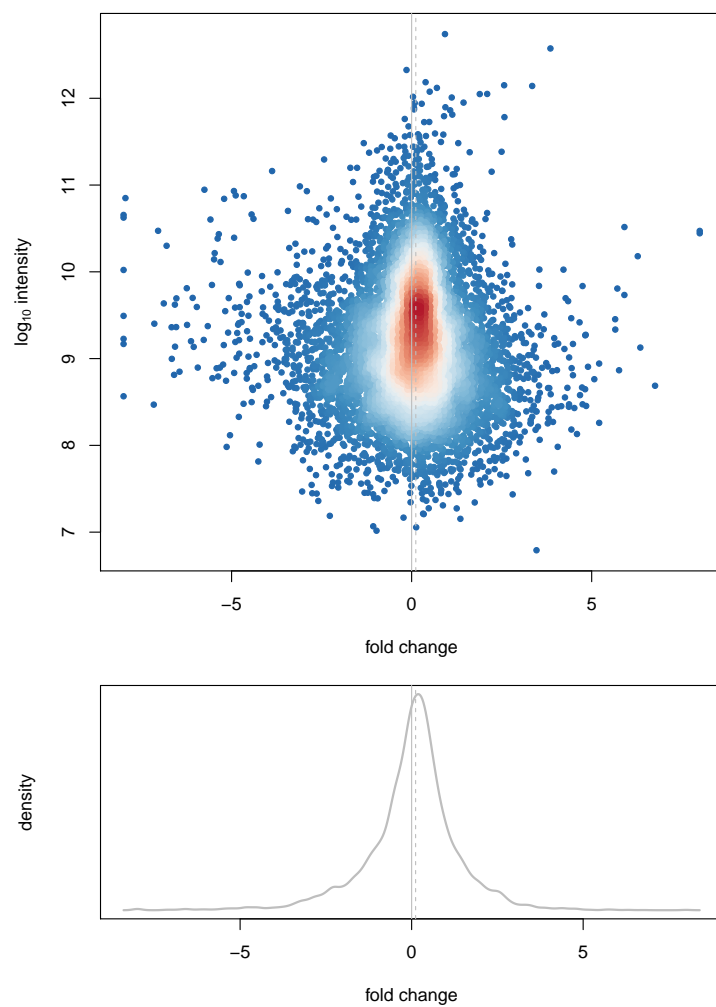


Figure 7: Fold changes of peptide abundances 2 and 3.  
 $\text{median}(\text{fc}) = 0.1159$        $\text{sd}(\text{fc}) = 1.3579$



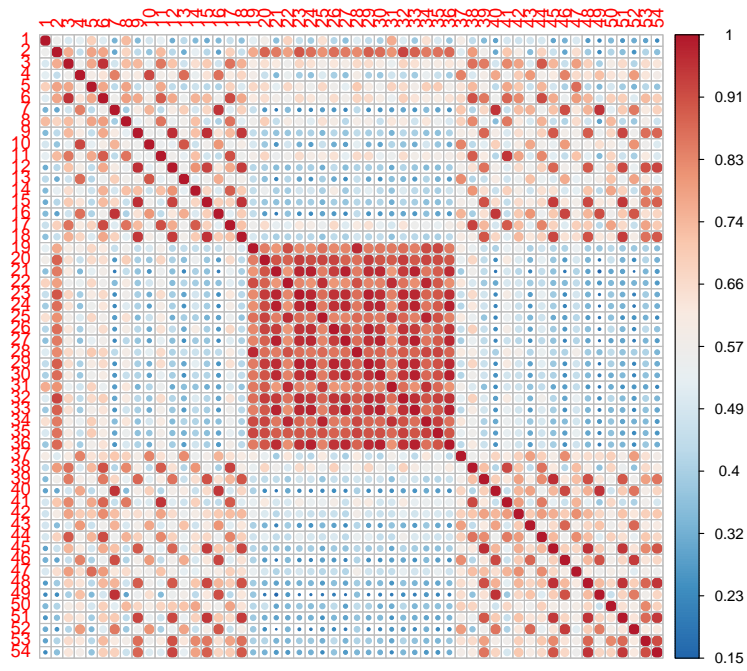


Figure 8: Pearson rank correlation of all peptide abundances. (min correlation = 0.1484, median correlation = 0.5701, max correlation = 1)

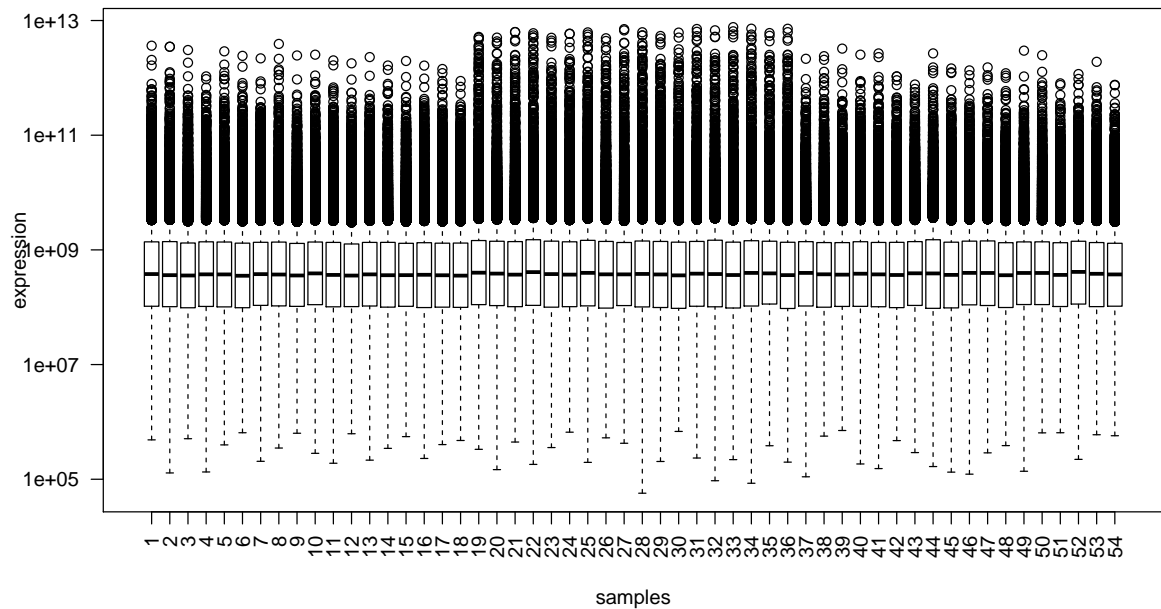


Figure 9: Boxplot of all peptide abundances.