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.

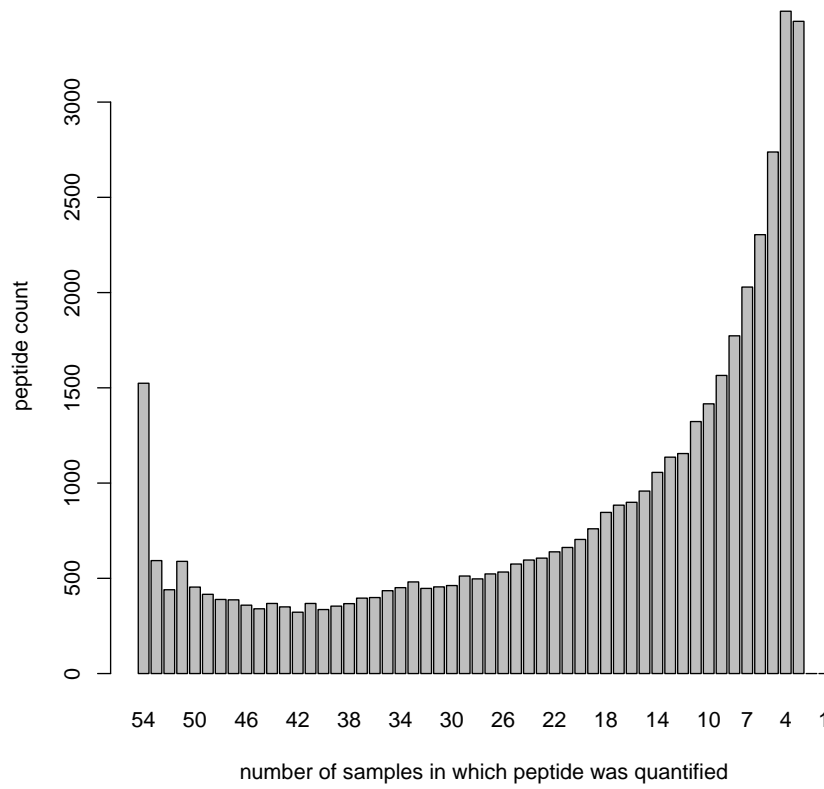| mod	specificity	number
Oxidation	M	8798
Methylthio	C	7927
Dioxidation	M	372
Label:13C(6)15N(4)	R	89
Label:13C(6)15N(2)	K	79

Table 4: Statistics of modifications.

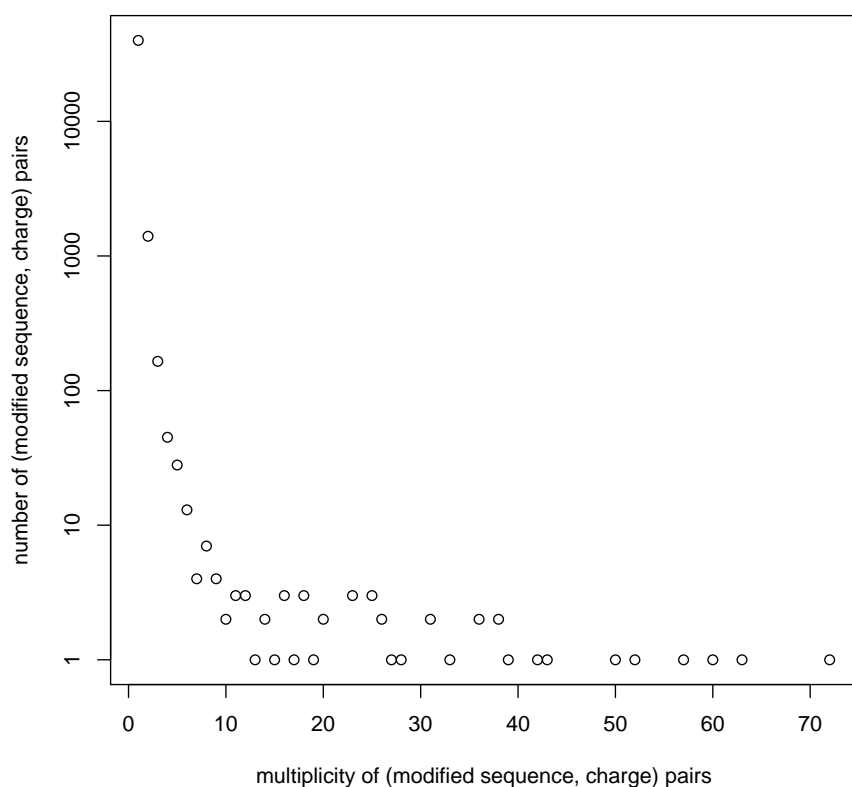Figure 1: Frequency plot of peptide quantifications.

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.
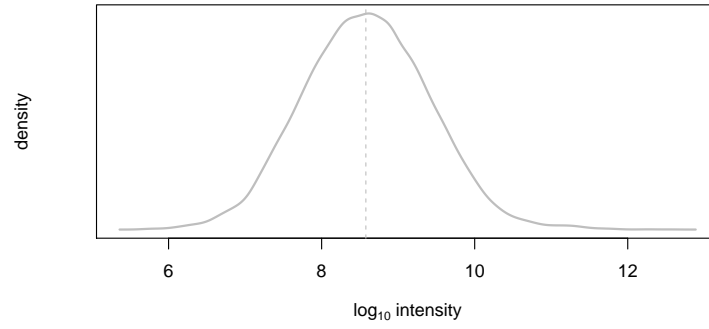
(a) peptide abundances 1, median(intensity) = $378, 509, 488$
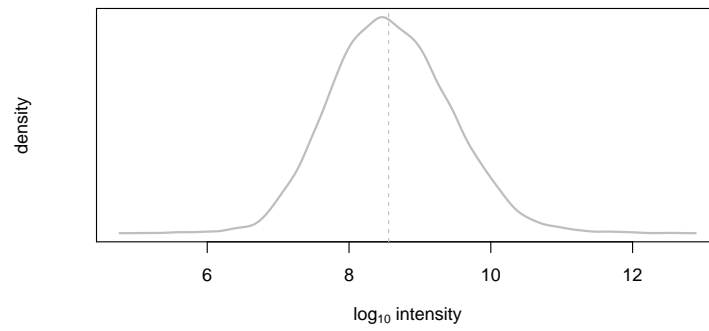
(b) peptide abundances 2, median(intensity) = $362, 260, 000$
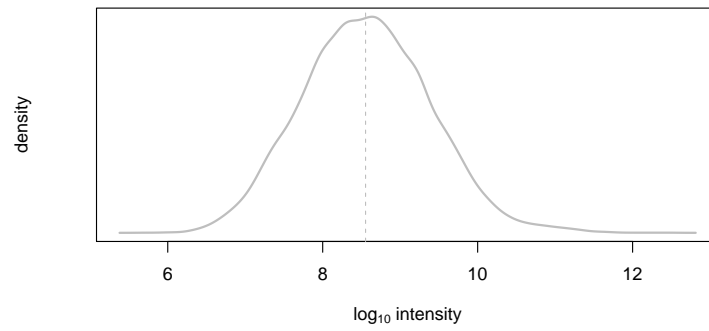
(c) peptide abundances 3, median(intensity) = $357, 520, 000$
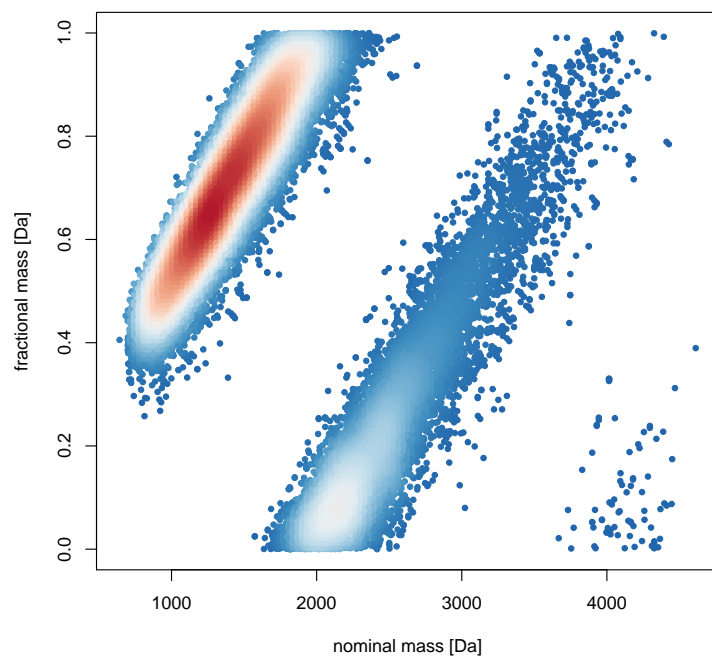
Figure 3: peptide abundance distributions.
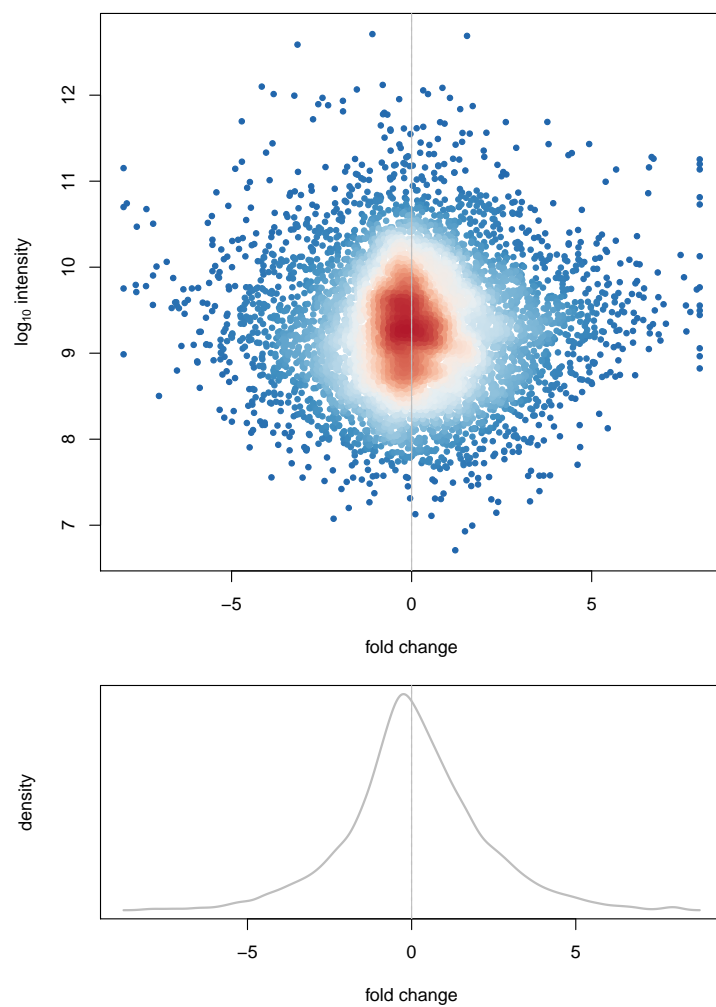
Figure 4: Kendrick nominal fractional mass plot

Figure 5: Fold changes of peptide abundances 1 and 2.
median(fc) = −0.0034   sd(fc) = 2.0759
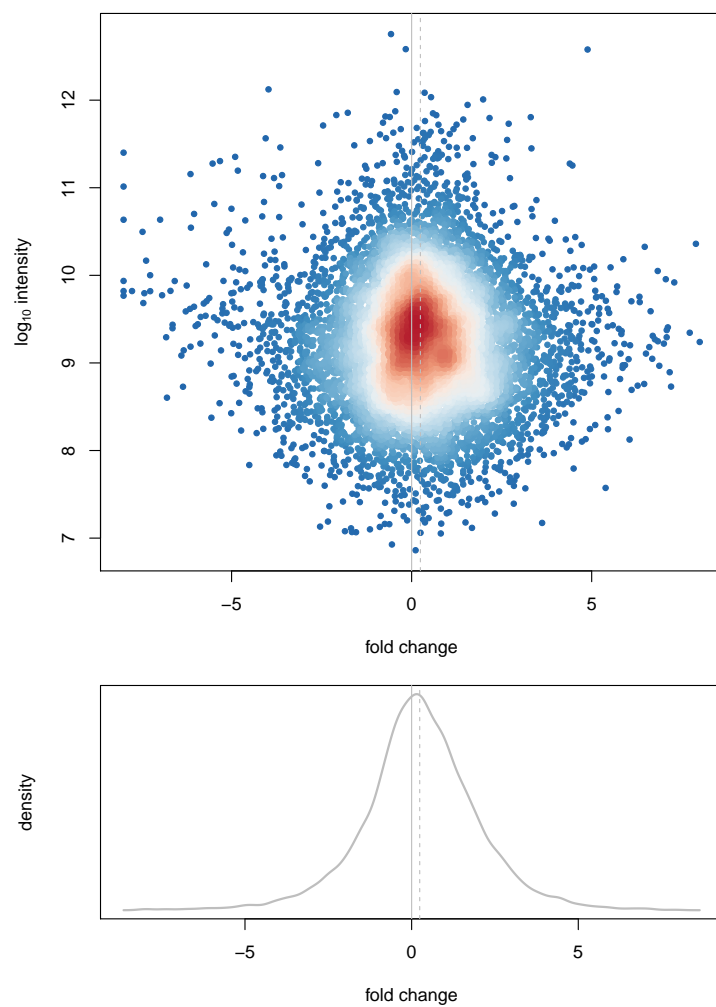
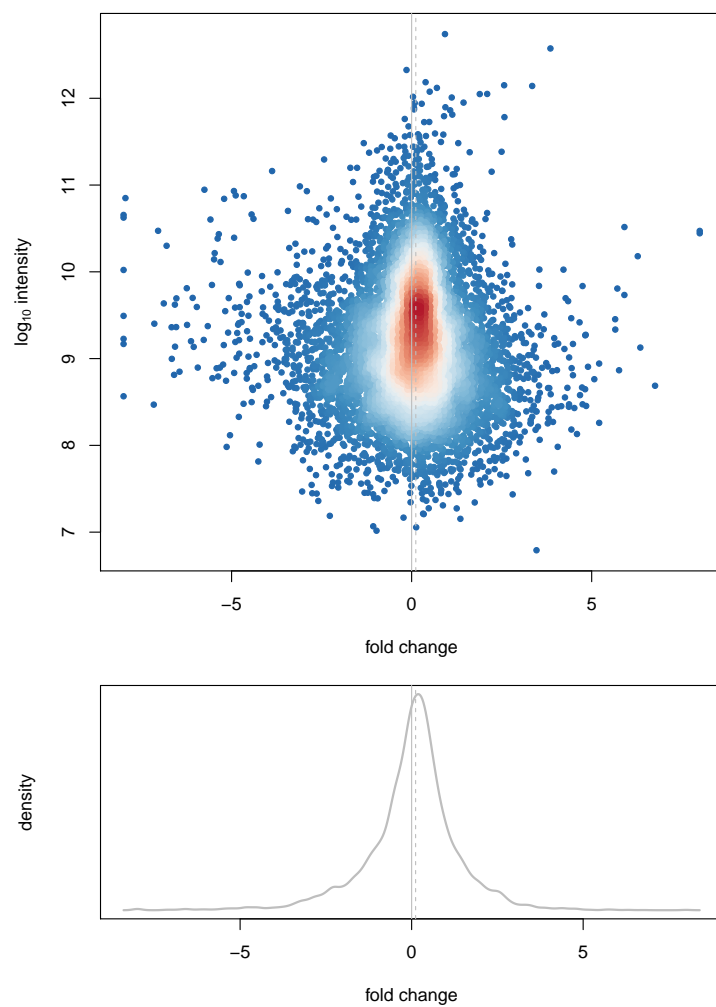Figure 6: Fold changes of peptide abundances 1 and 3.
median(fc) = 0.2428   sd(fc) = 1.7662

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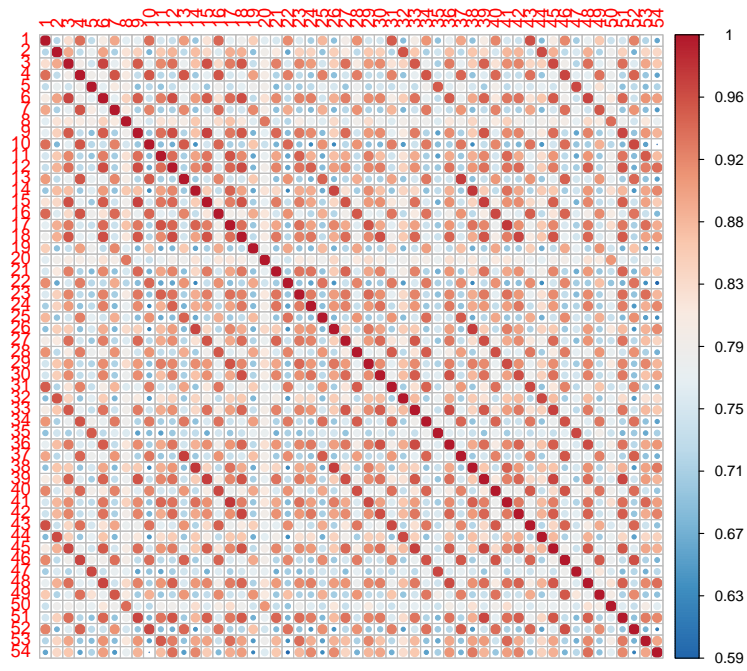median(fc) = 0.1159   sd(fc) = 1.3579

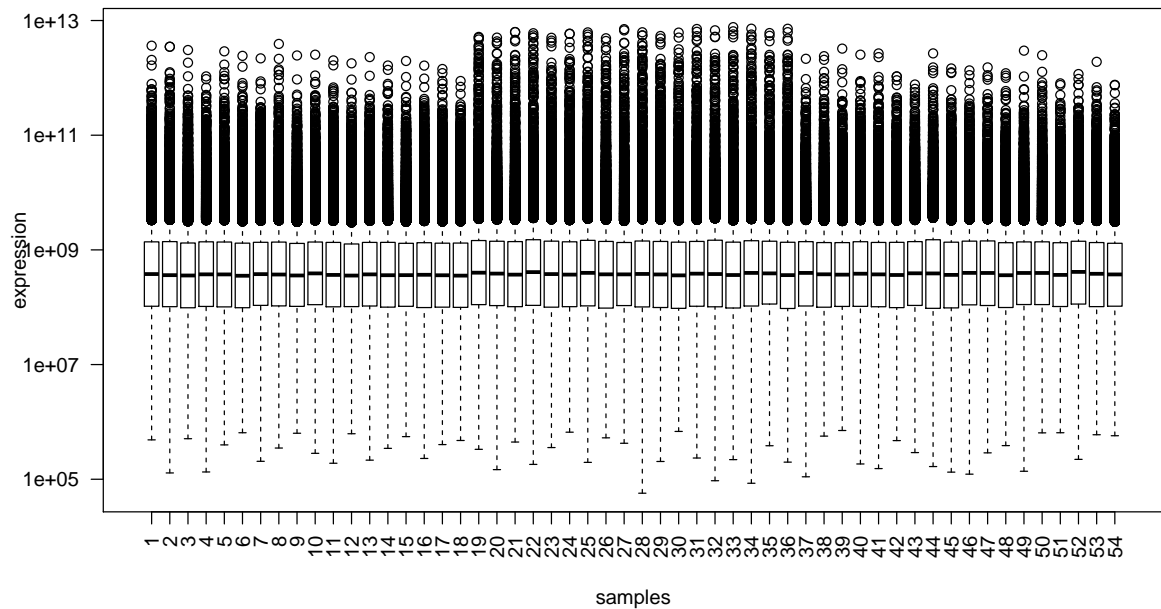Figure 8: Spearman rank correlation of all peptide abundances. (min correlation = 0.5873, median correlation = 0.8011, max correlation = 1)

Figure 9: Boxplot of all peptide abundances.