Report for PEP Section in mzTab File
example_4

The PEP section of the mzTab file contains $1,335$ quantified peptide features measured in 54 samples.

	number of peptides
quantified	1,335
identified (total)	1,335
identified (unique modified)	1,221
identified (unique stripped)	1,212

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.

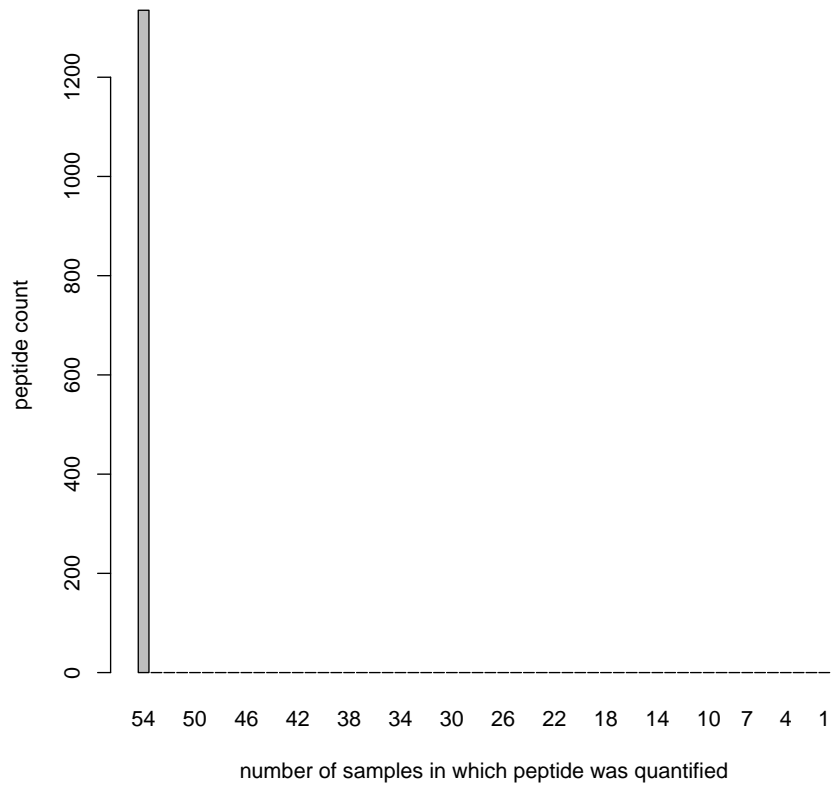| mod	specificity	number
Oxidation	M	179
Methylthio	C	150
Label:13C(6)15N(2)	K	6
Label:13C(6)15N(4)	R	4

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.
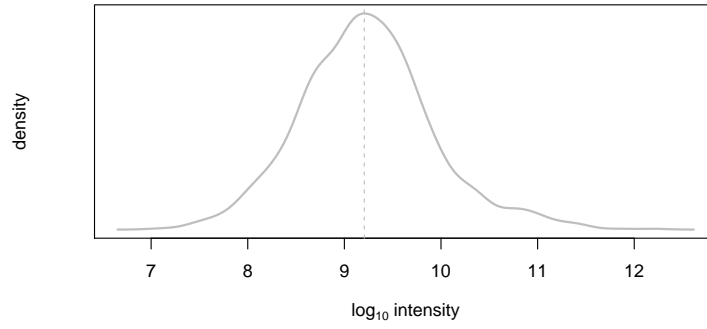
(a) peptide abundances 1, median(intensity) $= 1,605,469,952$
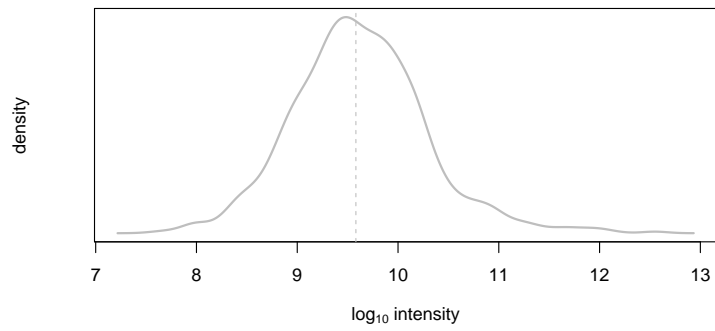
(b) peptide abundances 2, median(intensity) $= 3,819,539,968$
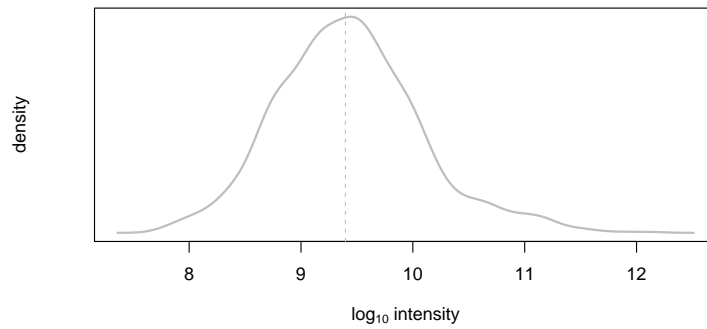
(c) peptide abundances 3, median(intensity) $= 2,497,959,936$

Figure 3: peptide abundance distributions.

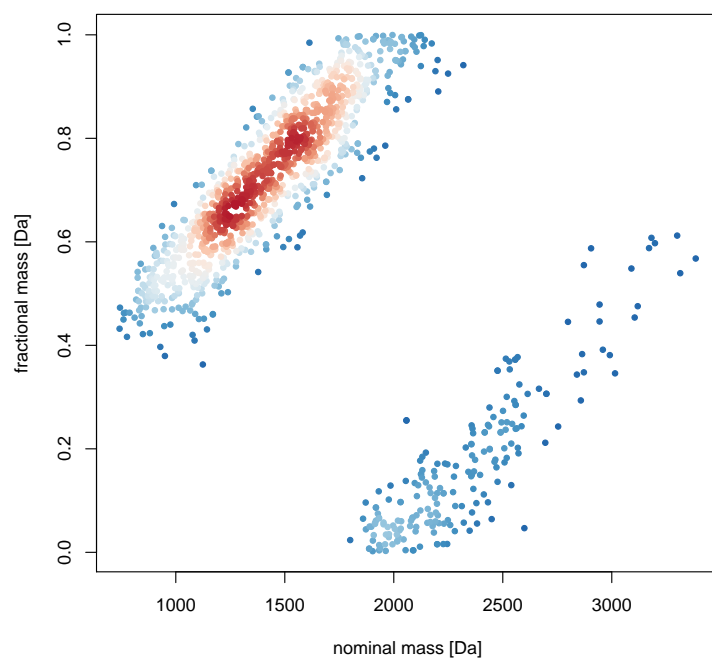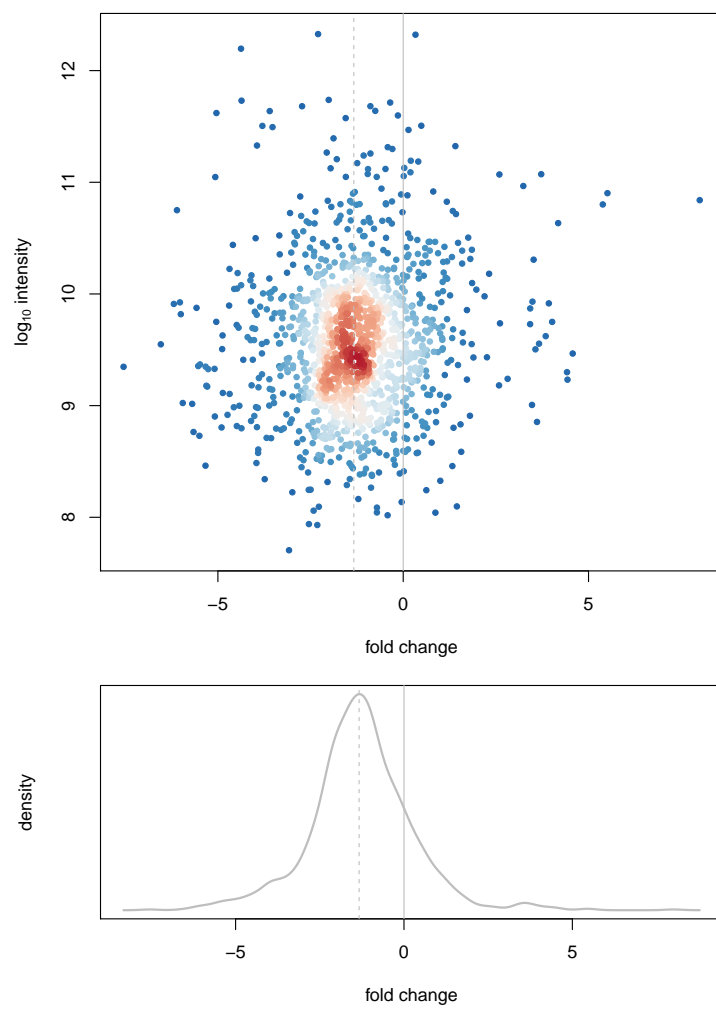Figure 4: Kendrick nominal fractional mass plot

Figure 5: Fold changes of peptide abundances 1 and 2.
median(fc) = −1.3328   sd(fc) = 1.5445
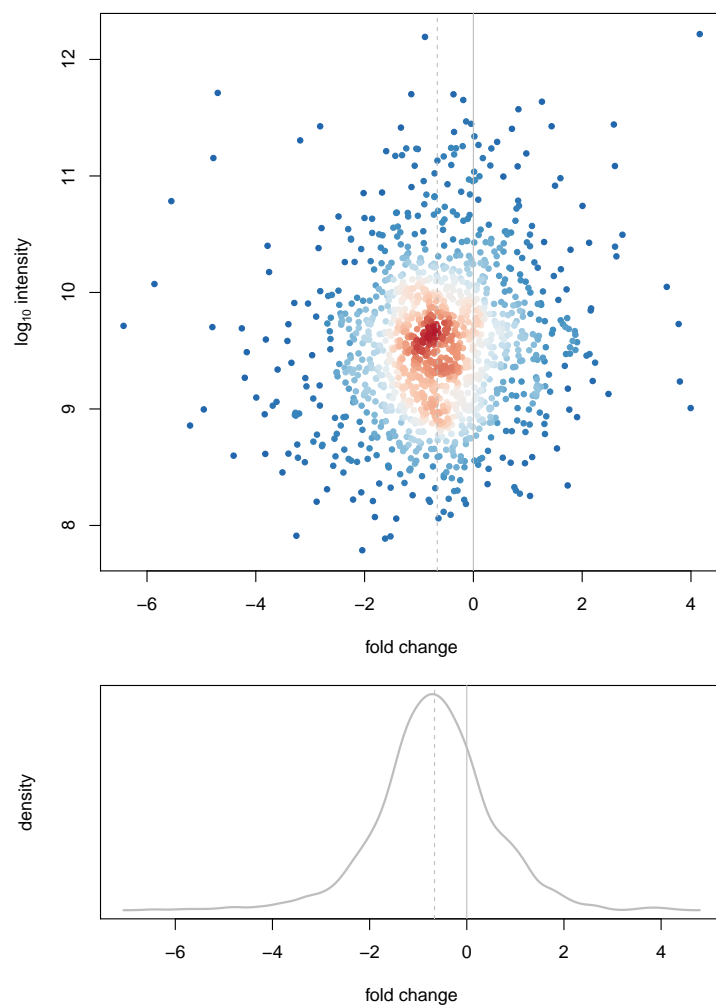
Figure 6: Fold changes of peptide abundances 1 and 3.
median(fc) = −0.6641   sd(fc) = 1.1804
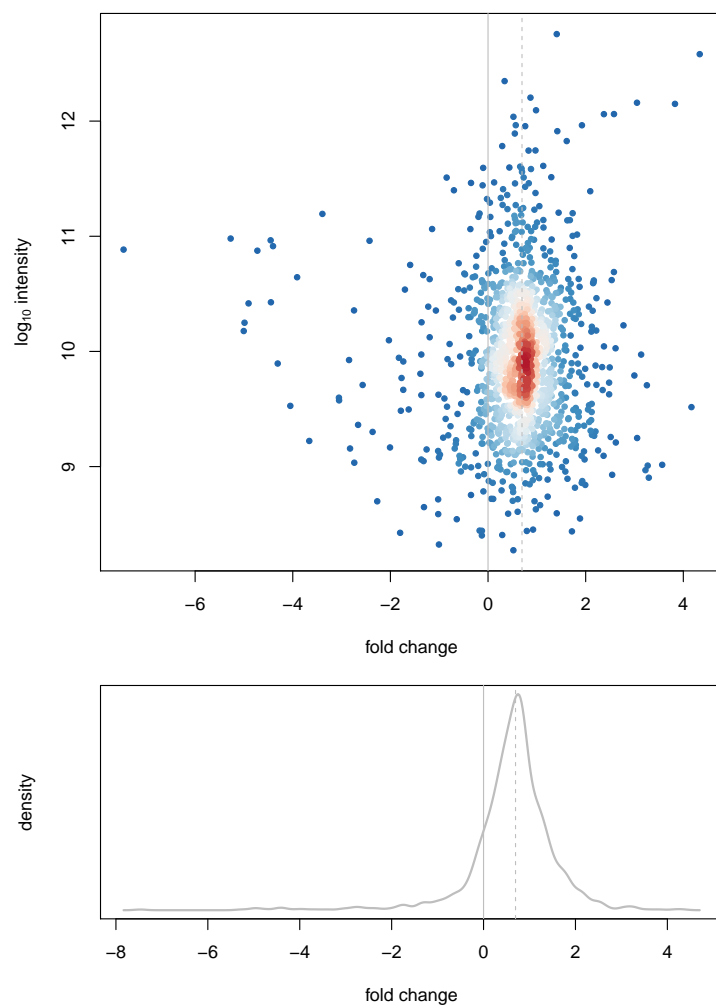
Figure 7: Fold changes of peptide abundances 2 and 3.
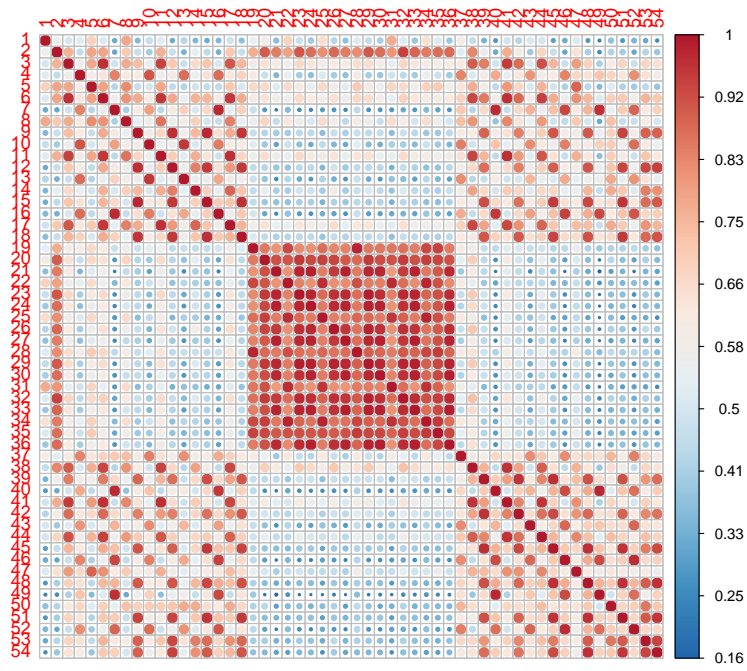median(fc) = 0.6958   sd(fc) = 0.9636

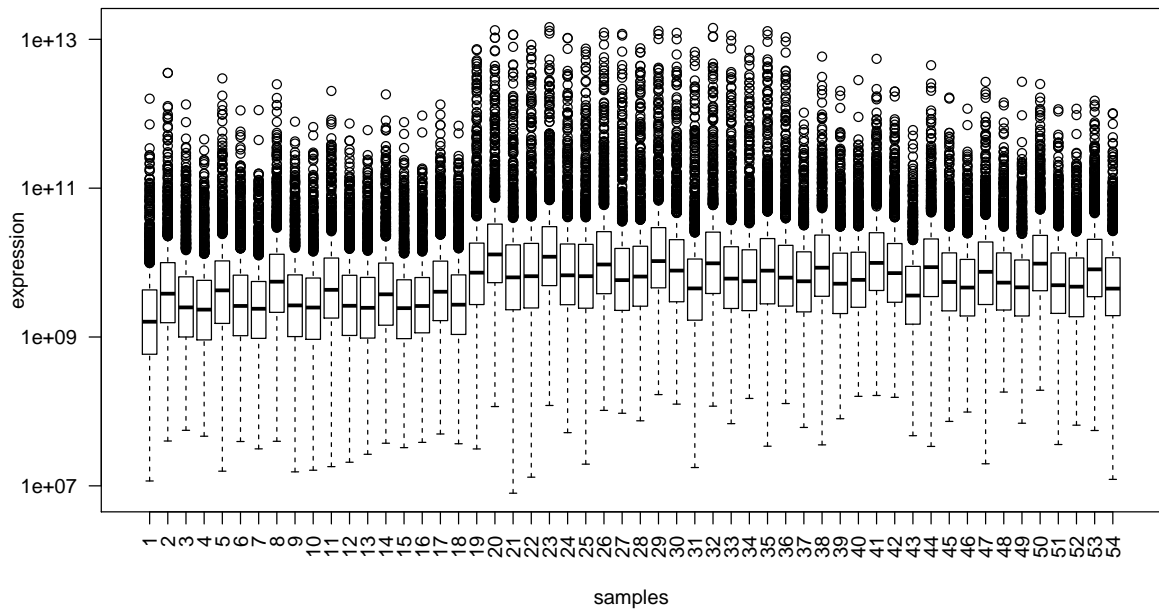Figure 8: Pearson correlation of all peptide abundances. (min correlation = 0.1622, median correlation = 0.5936, max correlation = 1)

Figure 9: Boxplot of all peptide abundances.