## 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              |
| identified (total)           | 2,160              |
| identified (unique modified) | 2,021              |
| identified (unique stripped) | 1,926              |

Table 1: Total number of quantified and identified peptides.

| mod             | specificity | $\operatorname{number}$ |
|-----------------|-------------|-------------------------|
| Carbamidomethyl | С           | 205                     |

Table 2: Statistics of modifications.

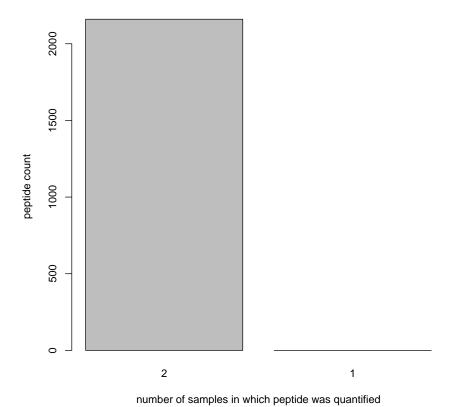


Figure 1: Frequency plot of peptide quantifications.

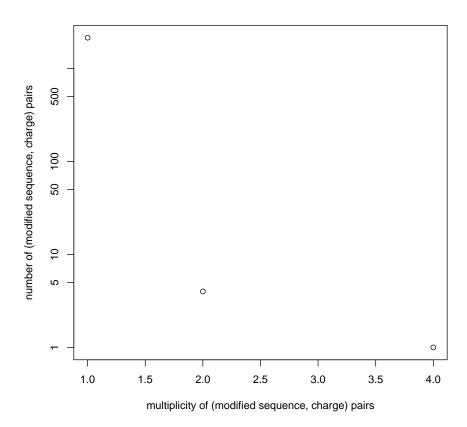
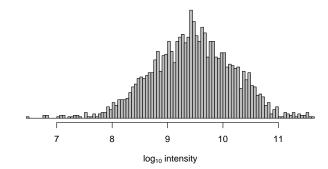


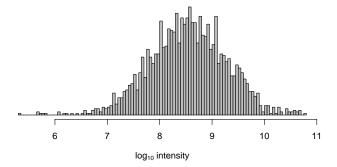
Figure 2: (modified sequence, charge) pair multiplicity vs frequency plot. Each peptide feature (characterised by a (possibly) modified peptide sequence and a charge state) should ideally occur only once in the analysis. In other words, peptides of multiplicity 1 should have a very high frequency. The 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) = 2,858,004,992

Visit



(b) peptide abundances 2, median (intensity) = 348,081,008

Figure 3: peptide abundance distributions.

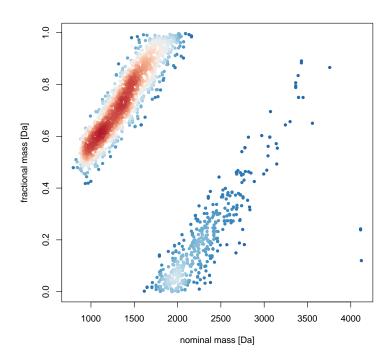


Figure 4: Kendrick nominal fractional mass plot

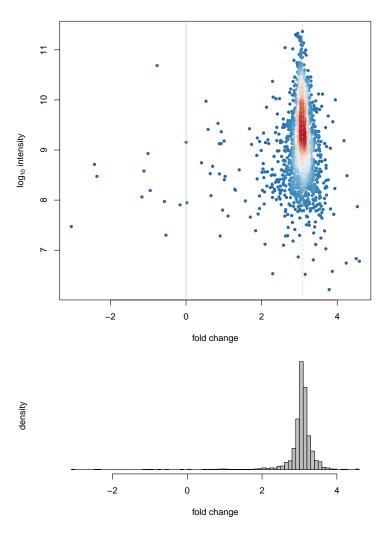


Figure 5: Fold changes of peptide abundances 1 and 2.  $median(fc) = 3.0739 \qquad sd(fc) = 0.4645$ 

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

Table 3: 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 | $\overline{\mathrm{m/z}}$ |
|-------------------|------------------------------|--------|----------------|---------------------------|
|                   | no matching accessions found |        |                |                           |

Table 4: Proteins of interest.