## 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%	
quantified (any zero)	0	0%	
quantified (any NaN)	0	0%	
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. (any zero) corresponds to peptides which are absent in one or more samples. (any NaN) corresponds to peptides which could not be quantified due to overlapping peptide features.

modification	specificity	number
no mods reported		

Table 2: Statistics of modifications.

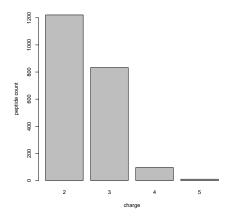


Figure 1: Charge distribution of peptide quantifications.

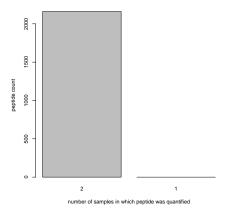


Figure 2: Frequency plot of peptide quantifications.

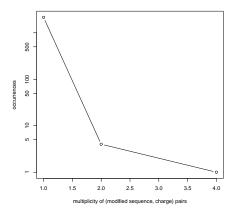


Figure 3: (modified sequence, charge) pair multiplicity vs frequency plot. Each peptide feature (characterised by a (possibly) modified peptide sequence and a charge state) should ideally occur only once in the analysis. In other words, peptides of multiplicity 1 should have a very high frequency. The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

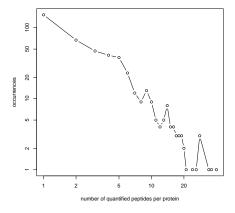


Figure 4: Number of quantified peptides per protein.

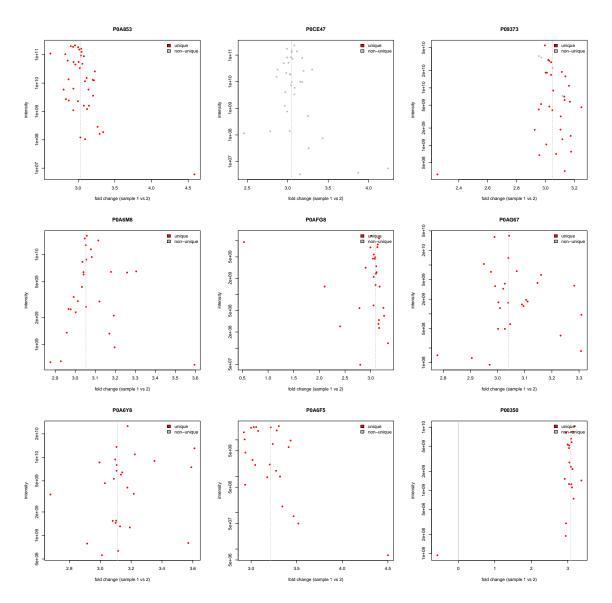
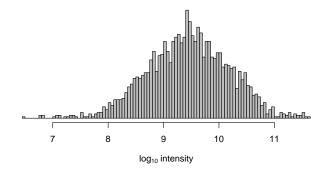


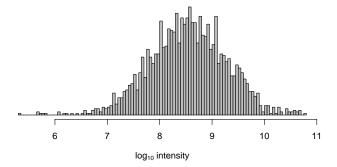
Figure 5: Fold changes of peptide abundances 1 and 2. For proteins with the largest number of quantified peptides.





(a) peptide abundances 1, median (intensity) = 2,858,004,992

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

Figure 6: peptide abundance distributions.

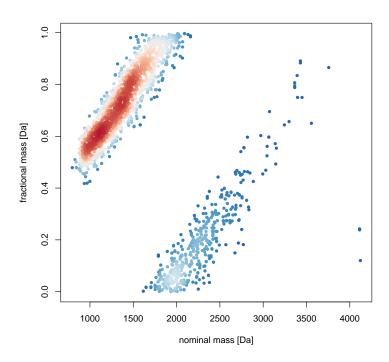


Figure 7: Kendrick nominal fractional mass plot

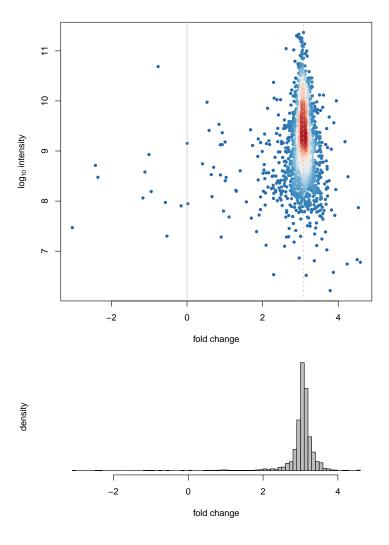


Figure 8: Fold changes of peptide abundances 1 and 2.  $median(fc) = 3.0739 \qquad sd(fc) = 0.4645$ 

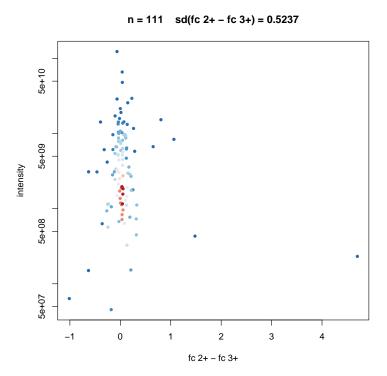


Figure 9: Fold changes of the same peptide in charge 2+ and 3+ are expected to be identical. Here we plot the difference of the 2+ and 3+ fold changes of sample 1 vs. sample 2 of all peptides which were identified and quantified in both charge states.

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

Table 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.