

## Report for PEP Section in mzTab File example\_3

The PEP section of the **mzTab** file contains 13,936 quantified peptide features measured in 3 samples.

	number of peptides	
quantified	13,936	100%
identified (total)	0	0%
identified (unique modified)	0	0%
identified (unique stripped)	0	0%

Table 1: Total number of quantified and identified peptides.

modification	specificity	number
no mods reported		

Table 2: Statistics of modifications.

sample	finite	zero	nan
1	13936	0	0
2	13936	0	0
3	13936	0	0

Table 3: Statistics of quantifications.

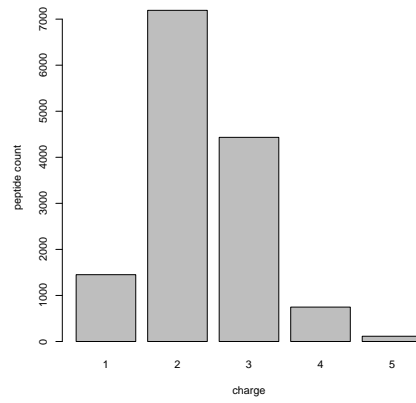


Figure 1: Charge distribution of peptide quantifications.

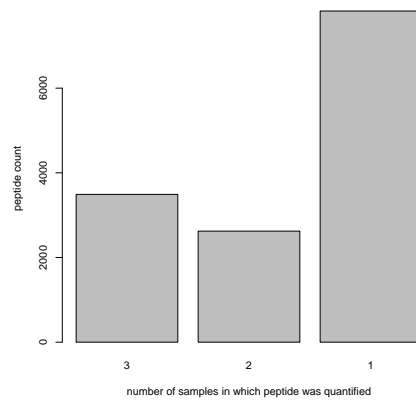
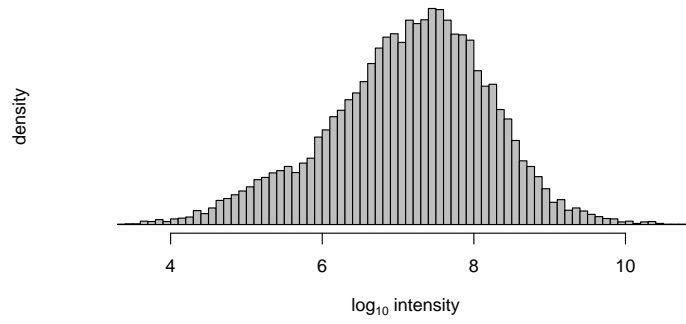
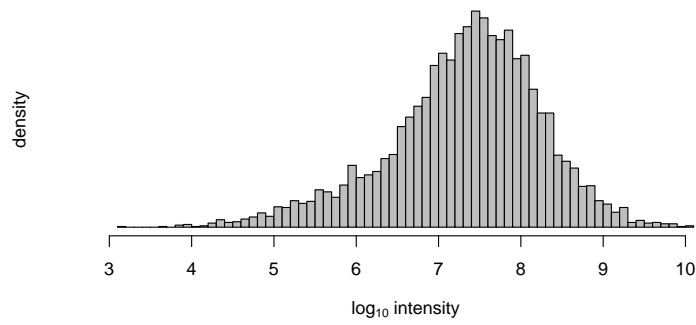


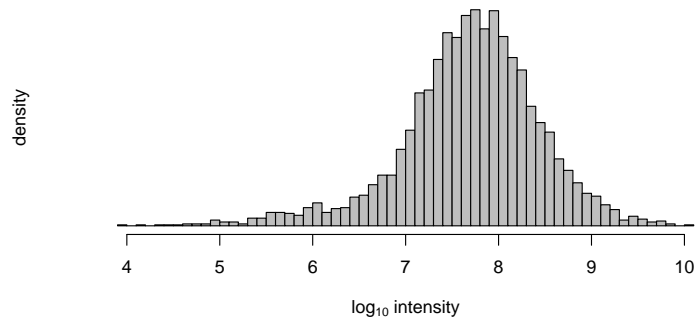
Figure 2: Frequency plot of peptide quantifications.



(a) peptide abundances 1, median(intensity) = 16,881,700



(b) peptide abundances 2, median(intensity) = 26,020,850



(c) peptide abundances 3, median(intensity) = 54,309,500

Figure 3: peptide abundance distributions.



Figure 4: Kendrick nominal fractional mass plot

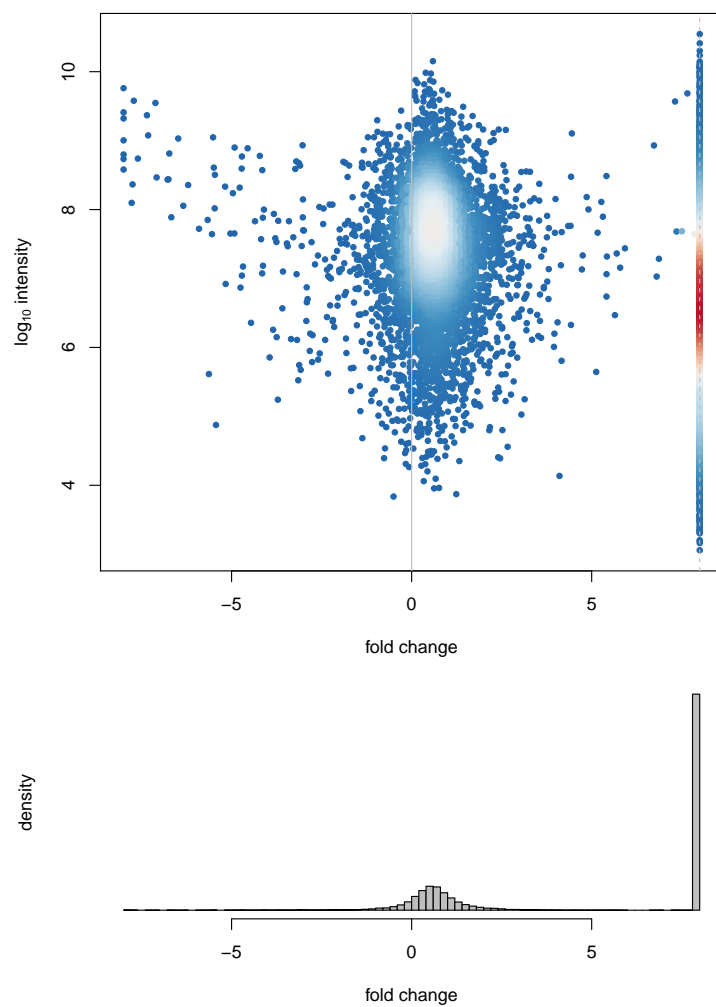


Figure 5: Fold changes of peptide abundances 1 and 2.  
 $\text{median}(\text{fc}) = 8$        $\text{sd}(\text{fc}) = 3.7588$

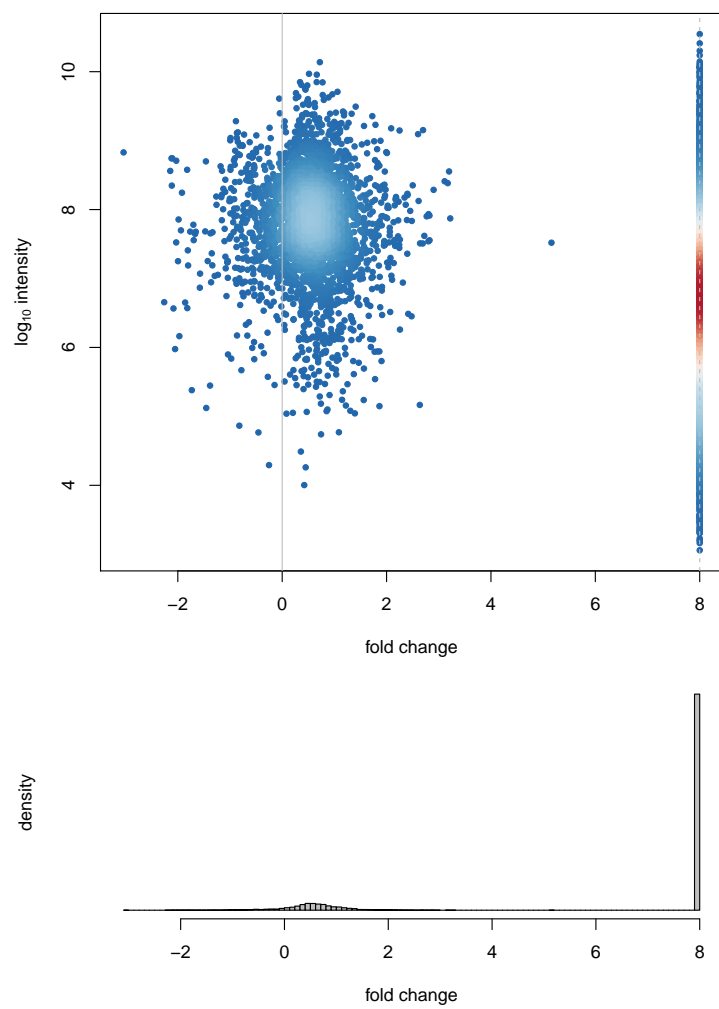


Figure 6: Fold changes of peptide abundances 1 and 3.  
 $\text{median}(\text{fc}) = 8$      $\text{sd}(\text{fc}) = 3.246$

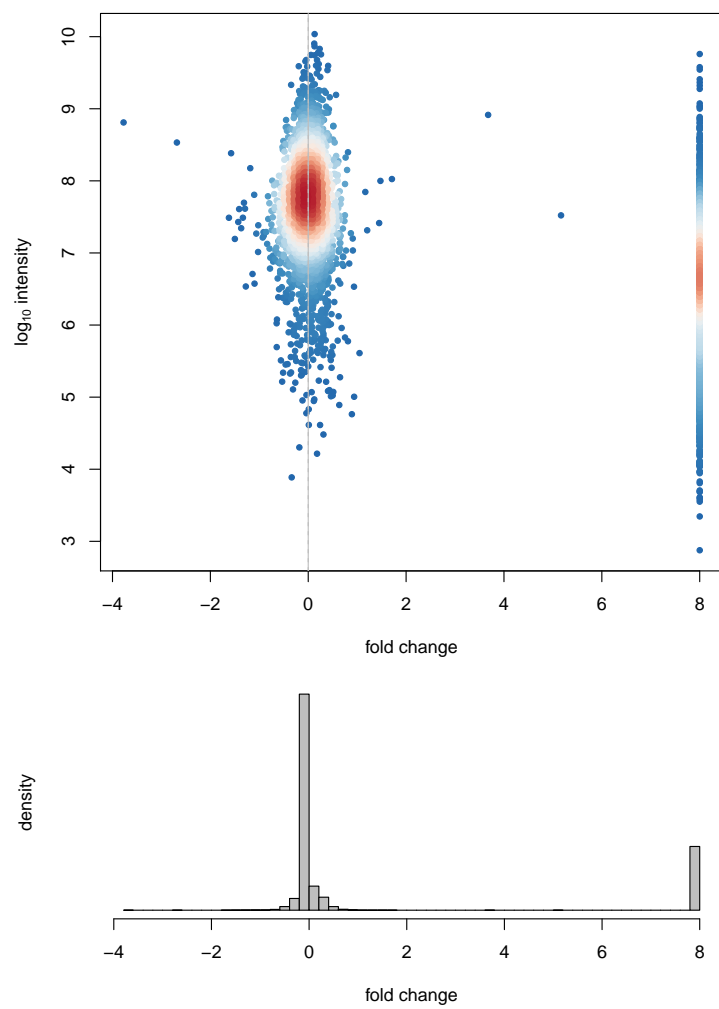


Figure 7: Fold changes of peptide abundances 2 and 3.  
 $\text{median}(\text{fc}) = 0$      $\text{sd}(\text{fc}) = 3.131$

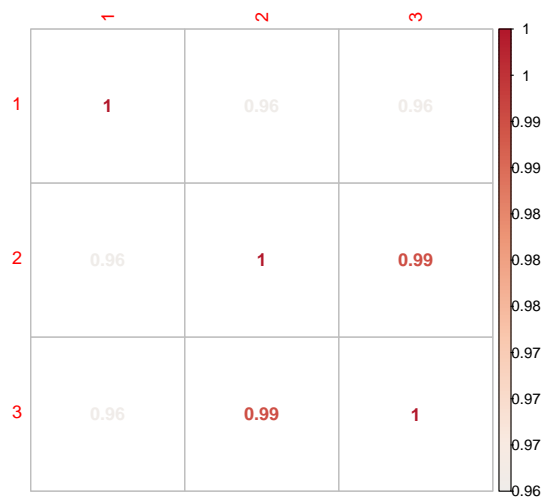


Figure 8: Pearson correlation of all peptide abundances. (min correlation = 0.962, median correlation = 0.9925, max correlation = 1)



Figure 9: Boxplot of all peptide abundances.



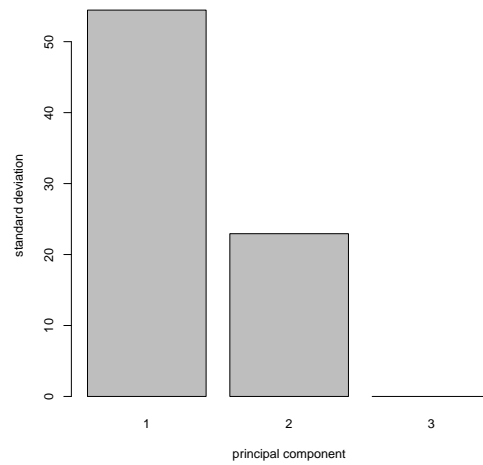


Figure 10: Standard deviation of all principal components.

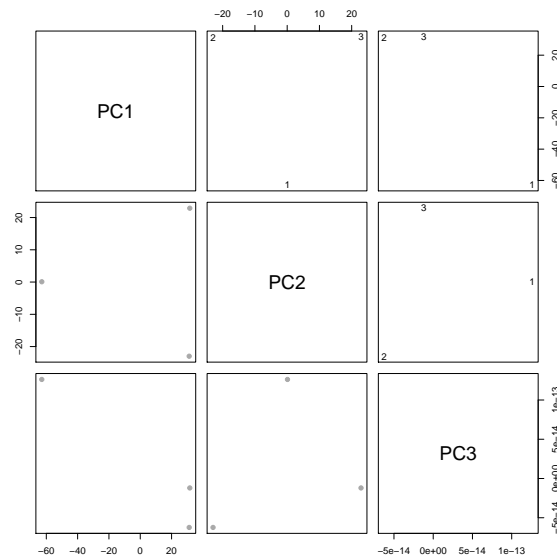


Figure 11: Principal Component Analysis of all peptides with complete quantifications. Any peptides with one or more missing values are ignored. The numbers in the upper right panels correspond to the sample IDs.

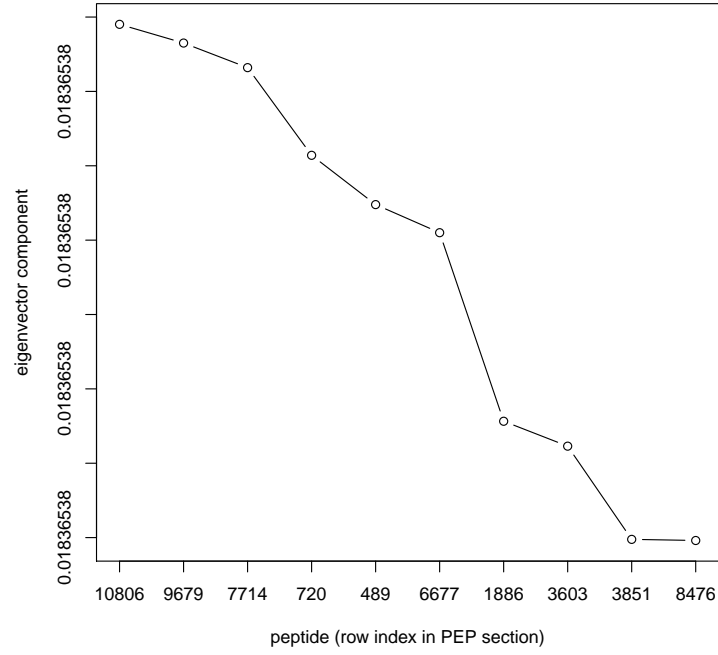


Figure 12: Most important contributions to the first principal component.

row index	modified sequence	accession	charge	retention time	m/z
10806			3	4932.93	612.65
9679			3	4552.35	865.12
7714			3	3890.40	749.71
720			3	1641.45	504.27
489			2	1501.44	907.41
6677			3	3578.85	510.25
1886			2	2104.85	673.27
3603			3	2620.65	446.21
3851			2	2696.46	847.41
8476			3	4135.46	590.95

Table 4: Most important contributions to the first principal component.

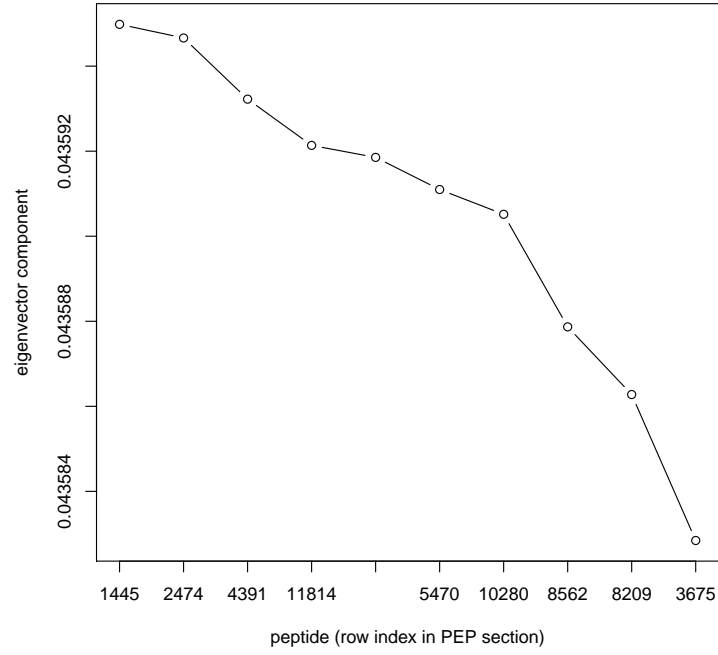


Figure 13: Most important contributions to the second principal component.

row index	modified sequence	accession	charge	retention time	m/z
1445			4	1960.07	393.93
2474			2	2290.57	651.85
4391			2	2875.15	732.32
11814			3	5437.40	754.06
12533			3	5735.98	754.06
5470			2	3213.90	911.98
10280			2	4746.62	1020.00
8562			2	4172.01	502.79
8209			3	4048.54	595.31
3675			2	2638.25	644.33

Table 5: Most important contributions to the second principal component.

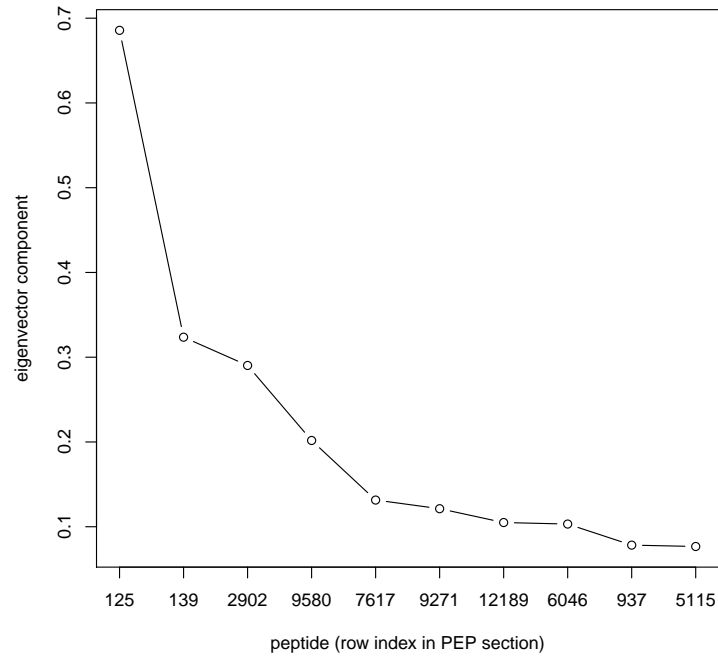


Figure 14: Most important contributions to the third principal component.

row index	modified sequence	accession	charge	retention time	m/z
125			4	1121.76	391.43
139			3	1143.65	521.58
2902			2	2424.37	512.26
9580			2	4519.87	623.30
7617			2	3861.43	557.29
9271			2	4411.47	725.40
12189			4	5610.30	656.61
6046			2	3393.82	453.74
937			2	1753.60	639.28
5115			2	3108.79	739.89

Table 6: Most important contributions to the third principal component.

modified sequence	accession	charge	retention time	m/z
no sequences reported				

Table 7: 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	m/z
no accessions reported				

Table 8: Proteins of interest.