

## 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
identified (total)	0
identified (unique modified)	0
identified (unique stripped)	0

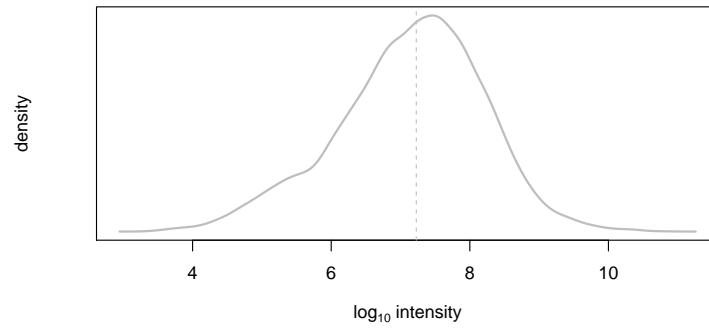
Table 1: Total number of quantified and identified peptides.

modification	specificity	number
no mods reported		

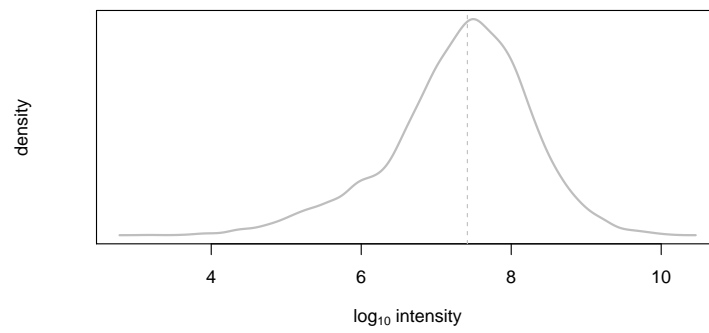
Table 2: Statistics of modifications.



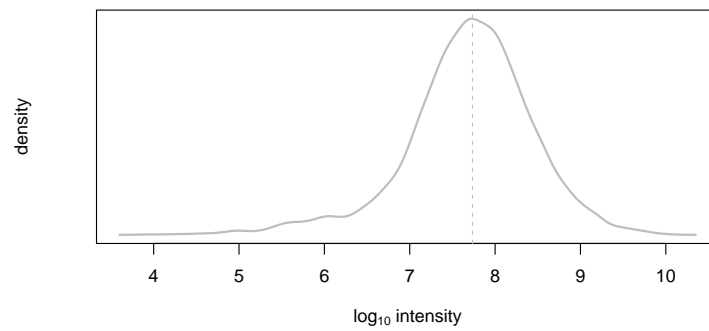
Figure 1: Frequency plot of peptide quantifications.



(a) peptide abundances 1,  $\text{median}(\text{intensity}) = 16,881,700$



(b) peptide abundances 2,  $\text{median}(\text{intensity}) = 26,020,850$



(c) peptide abundances 3,  $\text{median}(\text{intensity}) = 54,309,500$

Figure 2: peptide abundance distributions.



Figure 3: Kendrick nominal fractional mass plot

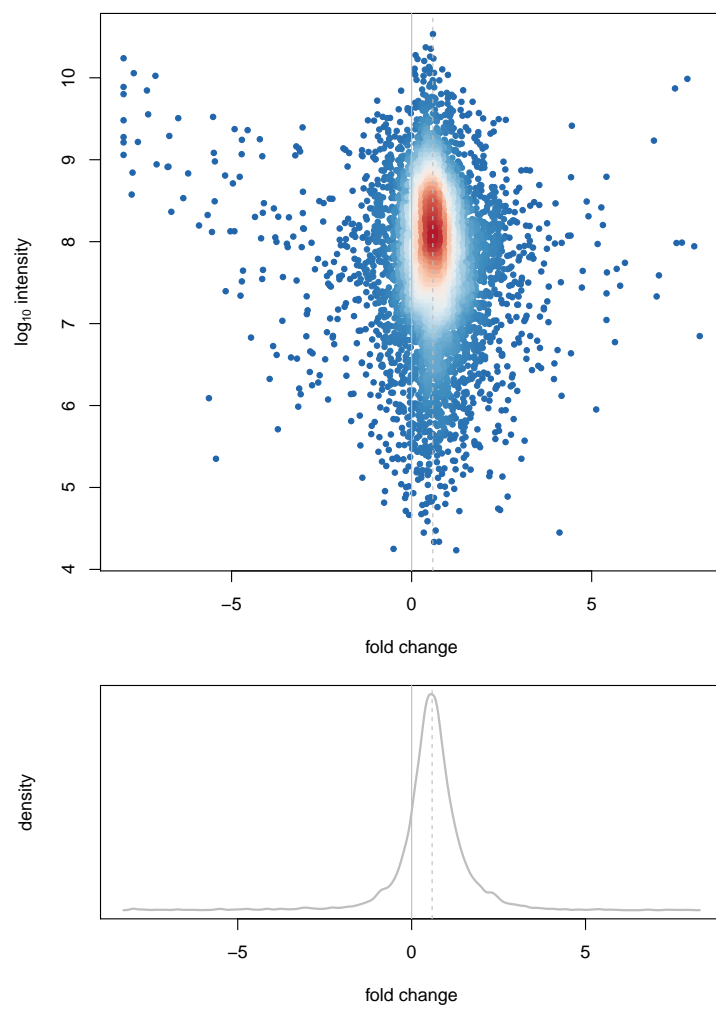


Figure 4: Fold changes of peptide abundances 1 and 2.  
 $\text{median}(\text{fc}) = 0.589$        $\text{sd}(\text{fc}) = 1.1158$

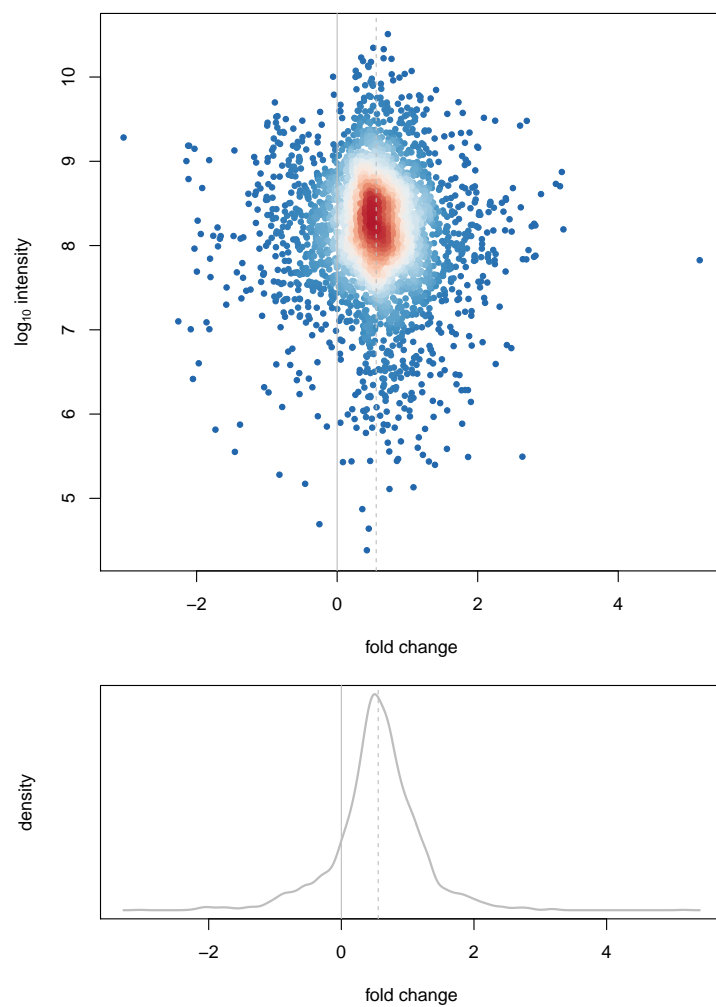


Figure 5: Fold changes of peptide abundances 1 and 3.  
 $\text{median}(\text{fc}) = 0.5559$        $\text{sd}(\text{fc}) = 0.6453$

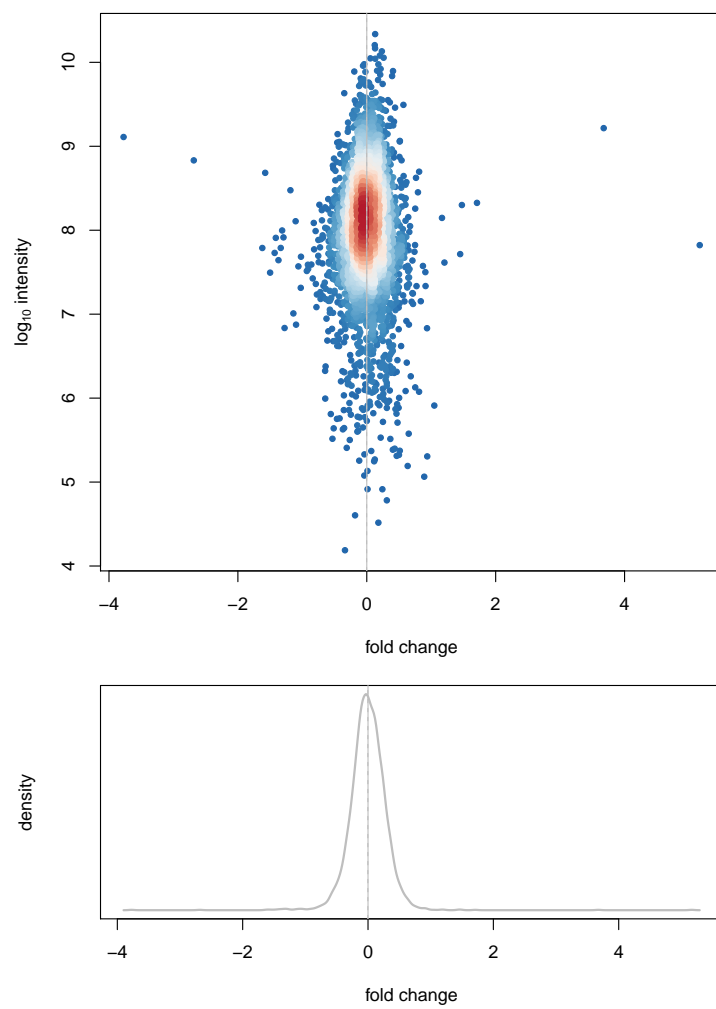


Figure 6: Fold changes of peptide abundances 2 and 3.  
 $\text{median}(\text{fc}) = -0.0025$        $\text{sd}(\text{fc}) = 0.3047$

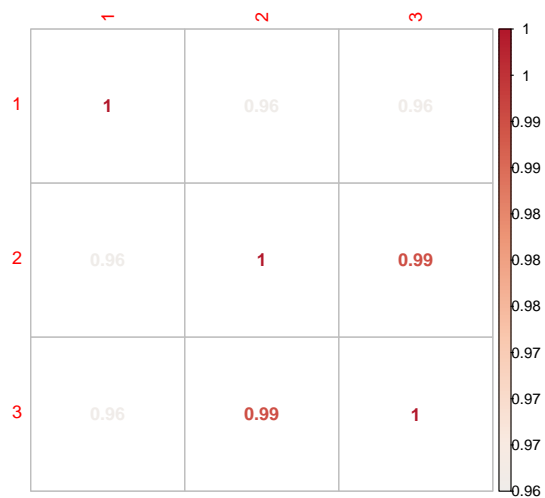


Figure 7: Pearson correlation of all peptide abundances. (min correlation = 0.962, median correlation = 0.9925, max correlation = 1)



Figure 8: Boxplot of all peptide abundances.



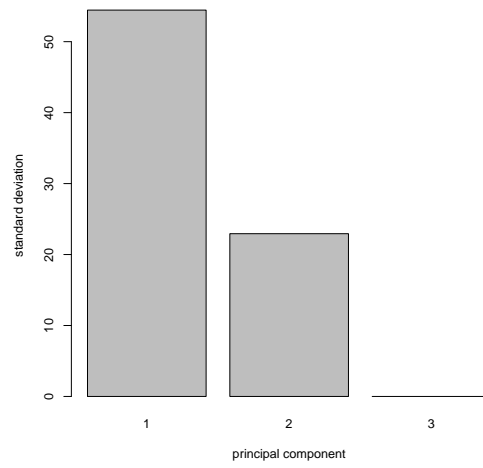


Figure 9: PCA components.

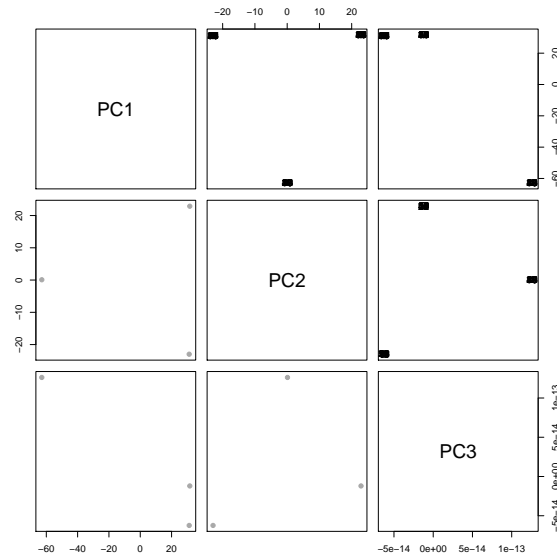


Figure 10: Principal Component Analysis of all peptides with complete quantifications. Any peptides with one or more missing values are ignored. The numbers in the upper right panels correspond to the sample IDs.

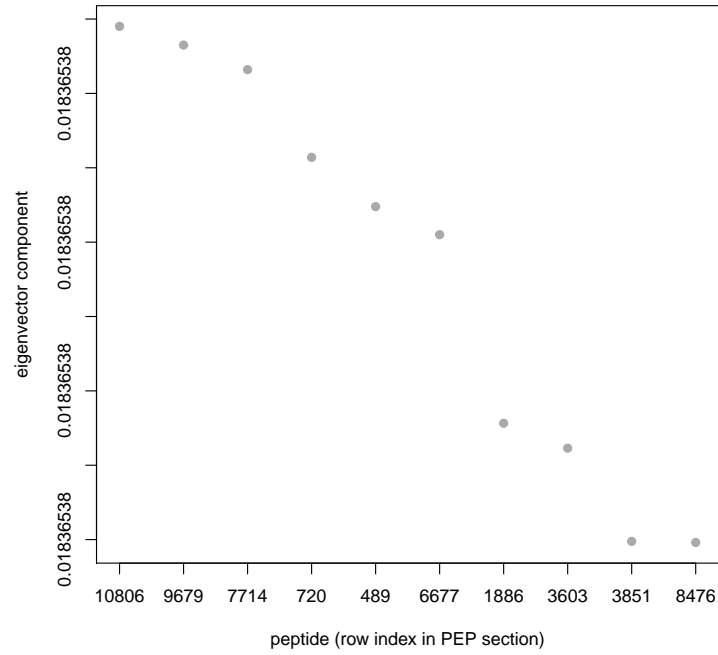


Figure 11: PCA 1st eigenvector.

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 3: PCA 1st eigenvector.

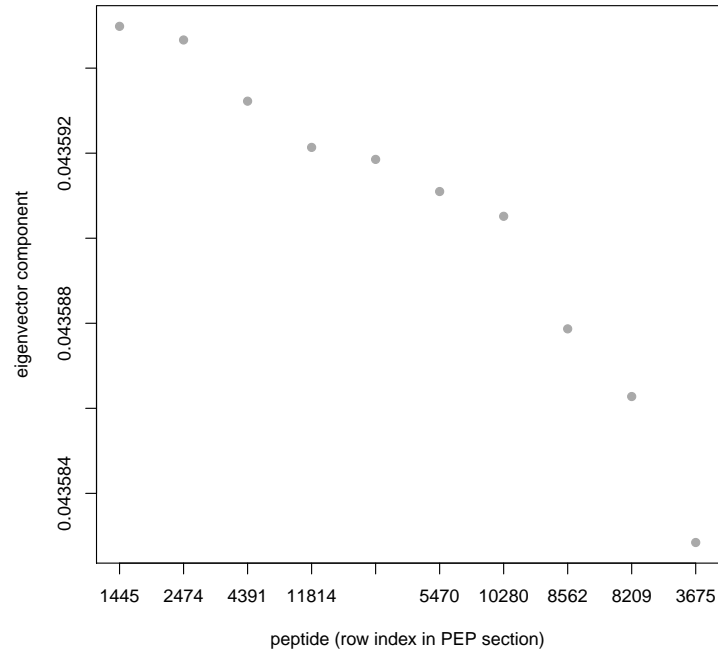


Figure 12: PCA 2nd eigenvector.

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 4: PCA 2nd eigenvector.

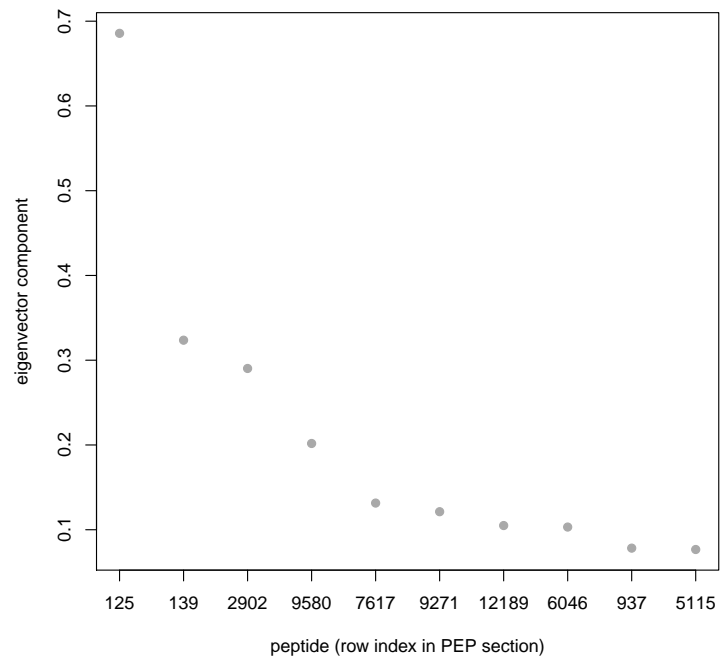


Figure 13: PCA 3rd eigenvector.

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 5: PCA 3rd eigenvector.

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

Table 6: 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 7: Proteins of interest.