

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 |

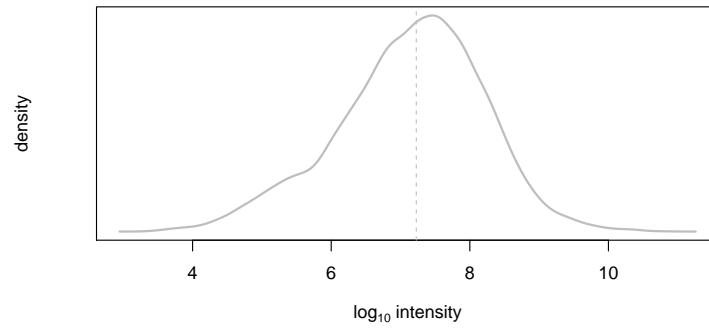
Table 1: Total number of quantified and identified peptides.

| modification | specificity | number |
|------------------|-------------|--------|
| no mods reported | | |

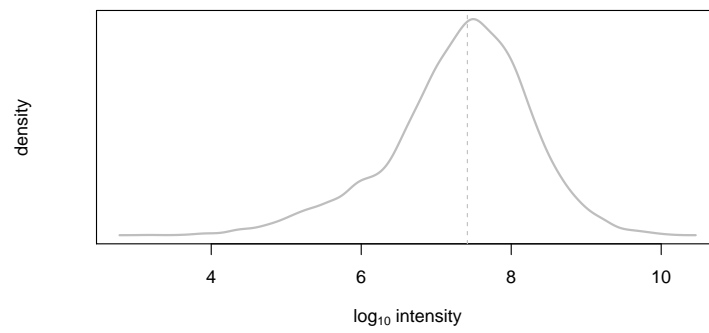
Table 2: Statistics of modifications.



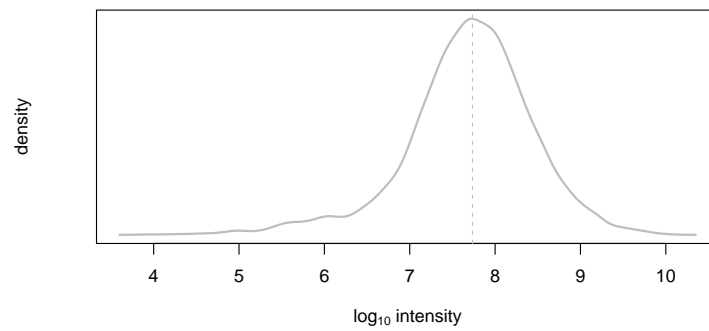
Figure 1: Frequency plot of peptide quantifications.



(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.

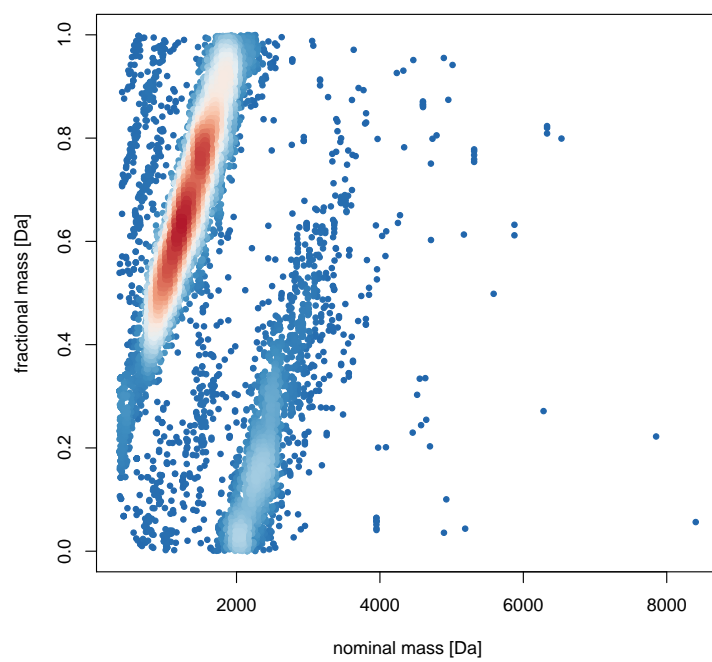


Figure 3: Kendrick nominal fractional mass plot

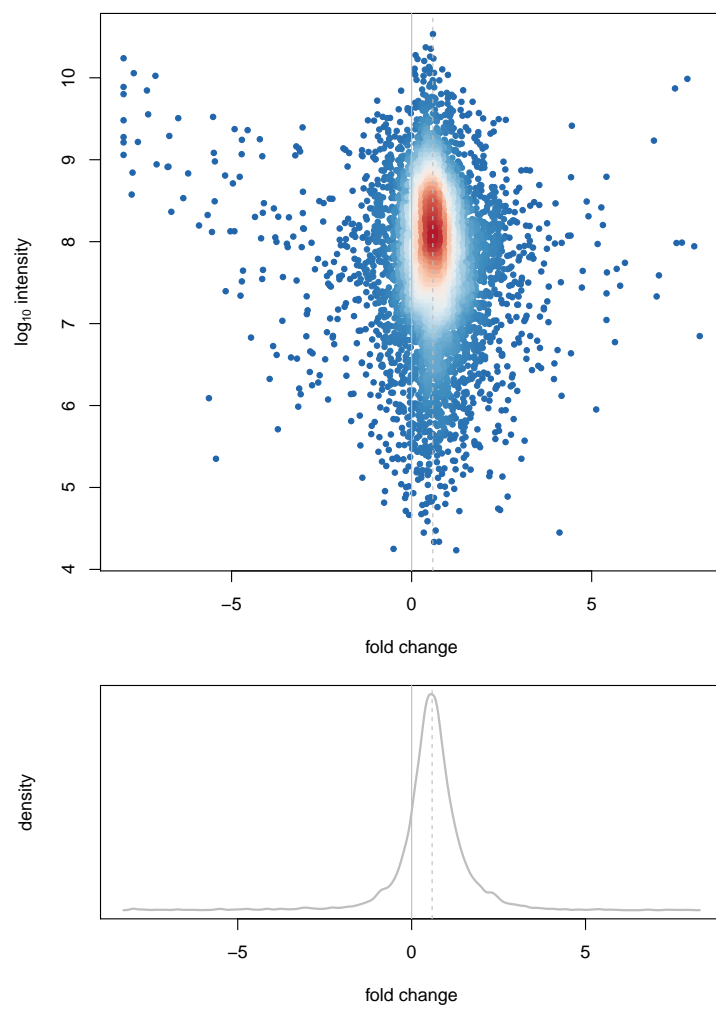


Figure 4: Fold changes of peptide abundances 1 and 2.
 $\text{median}(\text{fc}) = 0.589$ $\text{sd}(\text{fc}) = 1.1158$

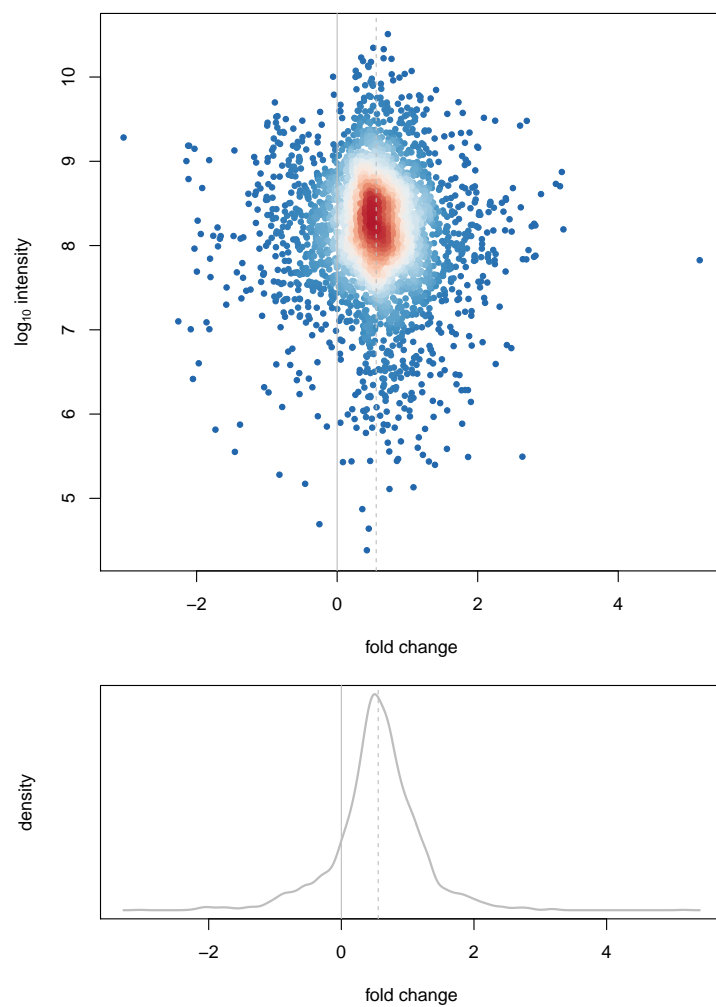


Figure 5: Fold changes of peptide abundances 1 and 3.
 $\text{median}(\text{fc}) = 0.5559$ $\text{sd}(\text{fc}) = 0.6453$

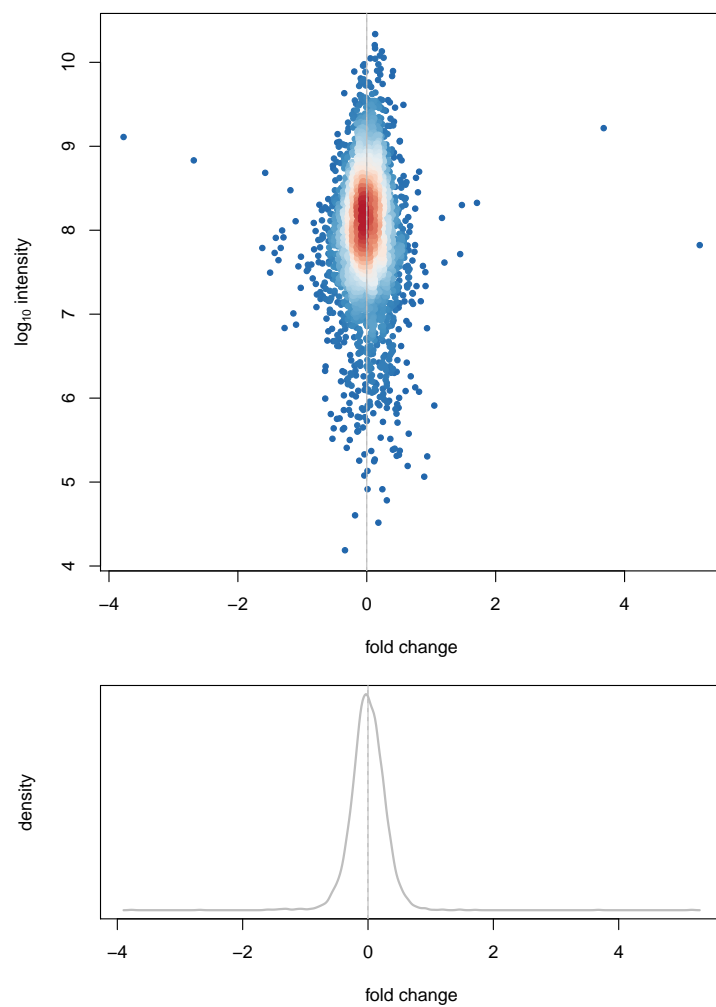


Figure 6: Fold changes of peptide abundances 2 and 3.
 $\text{median}(\text{fc}) = -0.0025$ $\text{sd}(\text{fc}) = 0.3047$

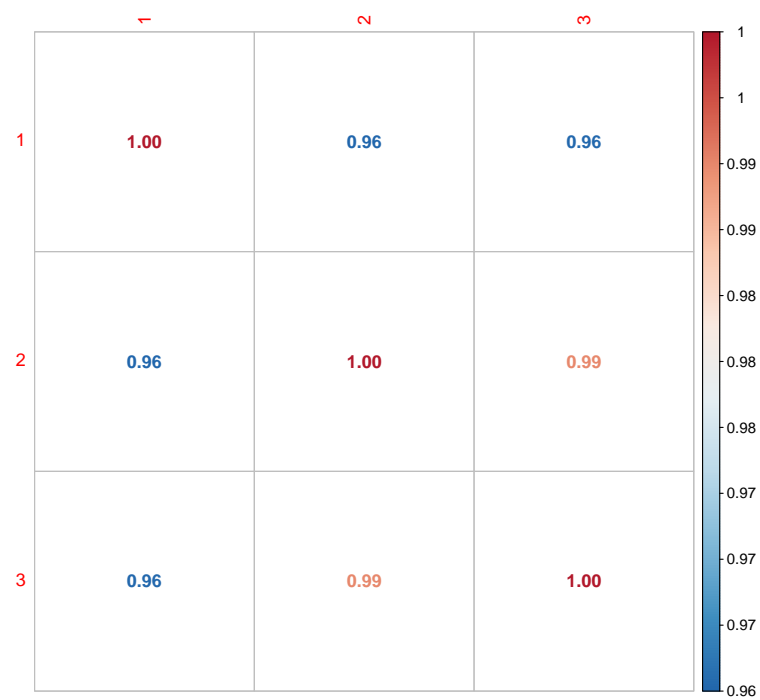


Figure 7: Pearson correlation of all peptide abundances. (min correlation = 0.962, median correlation = 0.9925, max correlation = 1)



Figure 8: Boxplot of all peptide abundances.

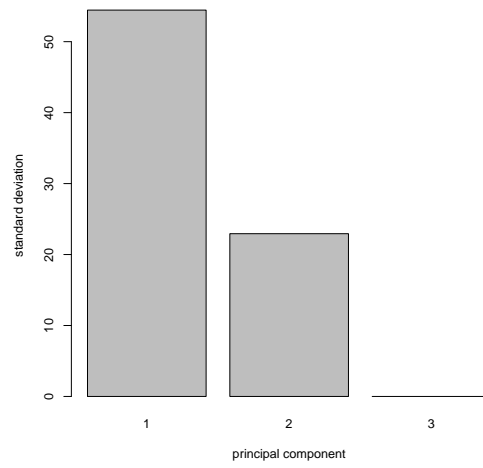


Figure 9: PCA components.

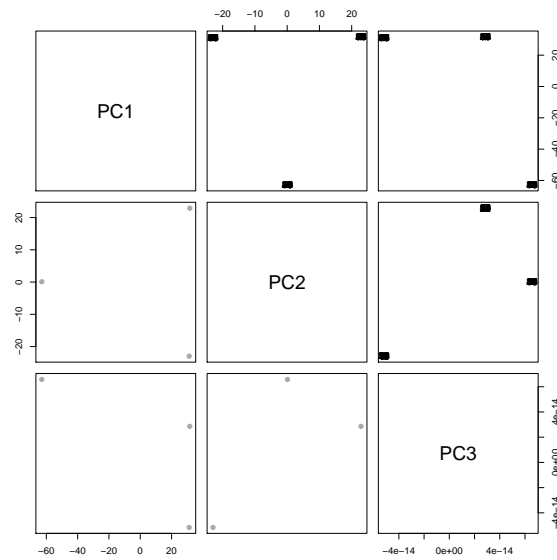


Figure 10: Principal Component Analysis of all peptides with complete quantifications. Any peptides with one or more missing values are ignored. The numbers in the upper right panels correspond to the sample IDs.

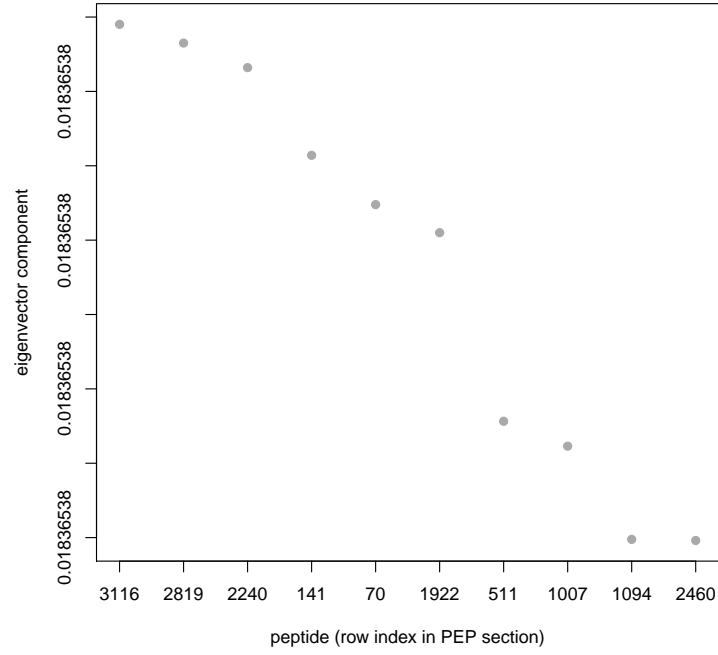


Figure 11: PCA 1st eigenvector.

| modified sequence | accession | charge | retention time | m/z |
|-------------------|-----------|--------|----------------|--------|
| | | 3 | 4932.93 | 612.65 |
| | | 3 | 4552.35 | 865.12 |
| | | 3 | 3890.40 | 749.71 |
| | | 3 | 1641.45 | 504.27 |
| | | 2 | 1501.44 | 907.41 |
| | | 3 | 3578.85 | 510.25 |
| | | 2 | 2104.85 | 673.27 |
| | | 3 | 2620.65 | 446.21 |
| | | 2 | 2696.46 | 847.41 |
| | | 3 | 4135.46 | 590.95 |

Table 3: PCA 1st eigenvector.

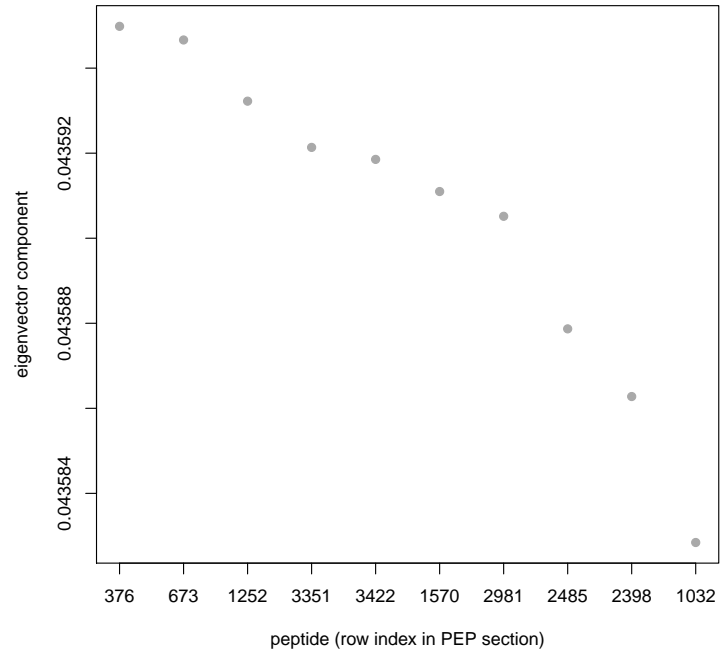


Figure 12: PCA 2nd eigenvector.

| modified sequence | accession | charge | retention time | m/z |
|-------------------|-----------|--------|----------------|---------|
| | | 4 | 1960.07 | 393.93 |
| | | 2 | 2290.57 | 651.85 |
| | | 2 | 2875.15 | 732.32 |
| | | 3 | 5437.40 | 754.06 |
| | | 3 | 5735.98 | 754.06 |
| | | 2 | 3213.90 | 911.98 |
| | | 2 | 4746.62 | 1020.00 |
| | | 2 | 4172.01 | 502.79 |
| | | 3 | 4048.54 | 595.31 |
| | | 2 | 2638.25 | 644.33 |

Table 4: PCA 2nd eigenvector.

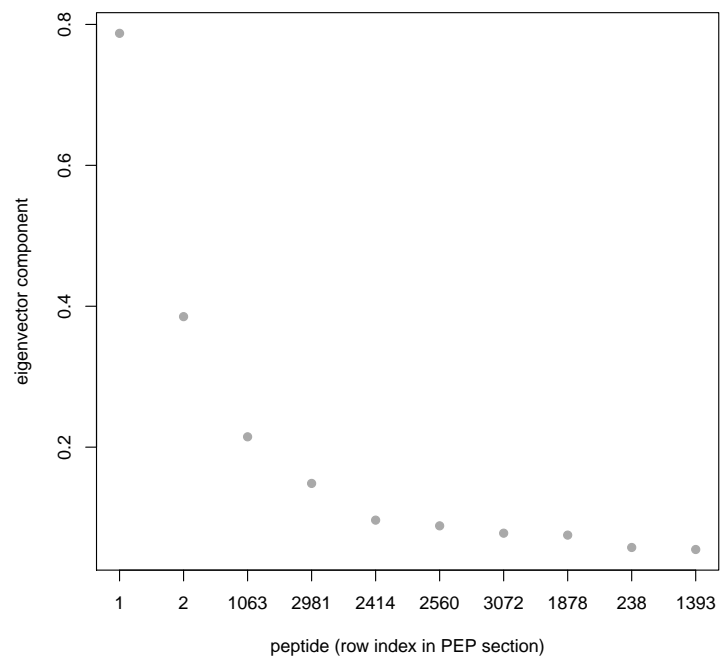


Figure 13: PCA 3rd eigenvector.

| modified sequence | accession | charge | retention time | m/z |
|-------------------|-----------|--------|----------------|---------|
| | | 4 | 1121.76 | 391.43 |
| | | 3 | 1143.65 | 521.58 |
| | | 2 | 2662.68 | 805.90 |
| | | 2 | 4746.62 | 1020.00 |
| | | 1 | 4073.04 | 1253.62 |
| | | 3 | 4246.42 | 788.77 |
| | | 2 | 4861.33 | 886.40 |
| | | 2 | 3542.95 | 924.41 |
| | | 3 | 1789.10 | 533.94 |
| | | 2 | 3002.91 | 808.93 |

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.