

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% |
| quantified (any zero) | 10,445 | 74.95% |
| quantified (any NaN) | 0 | 0% |
| identified (total) | 0 | 0% |
| identified (unique modified) | 0 | 0% |
| identified (unique stripped) | 0 | 0% |

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.

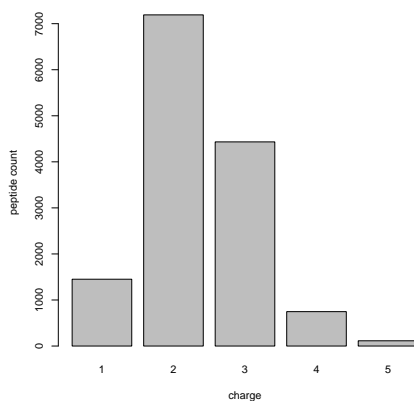


Figure 1: Charge distribution of peptide quantifications.

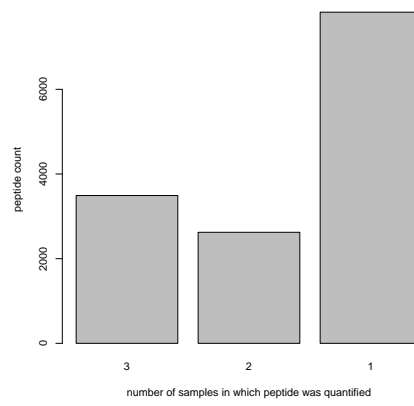
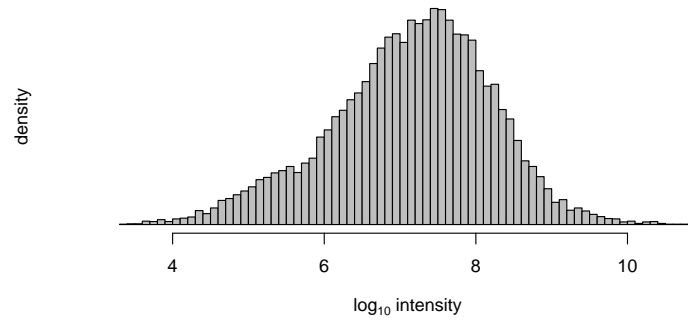
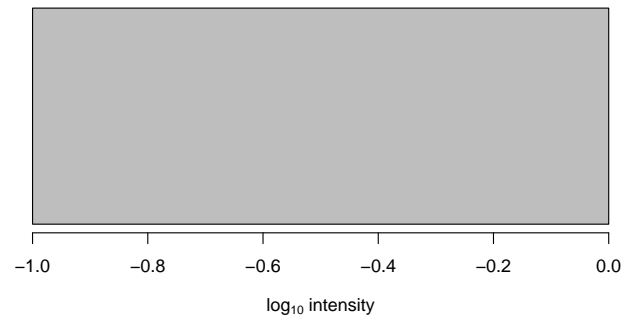


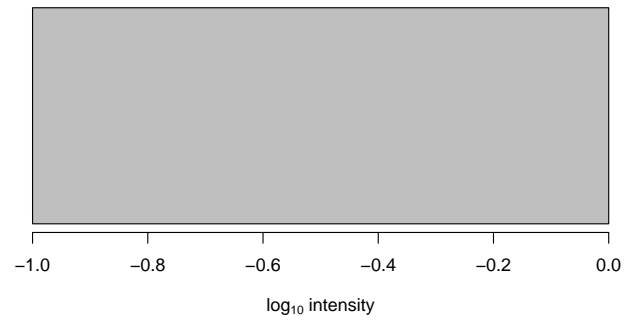
Figure 2: Frequency plot of peptide quantifications.



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



(b) peptide abundances 2, $\text{median}(\text{intensity}) = 1$



(c) peptide abundances 3, $\text{median}(\text{intensity}) = \text{TRUE}$

Figure 3: peptide abundance distributions.



Figure 4: Kendrick nominal fractional mass plot

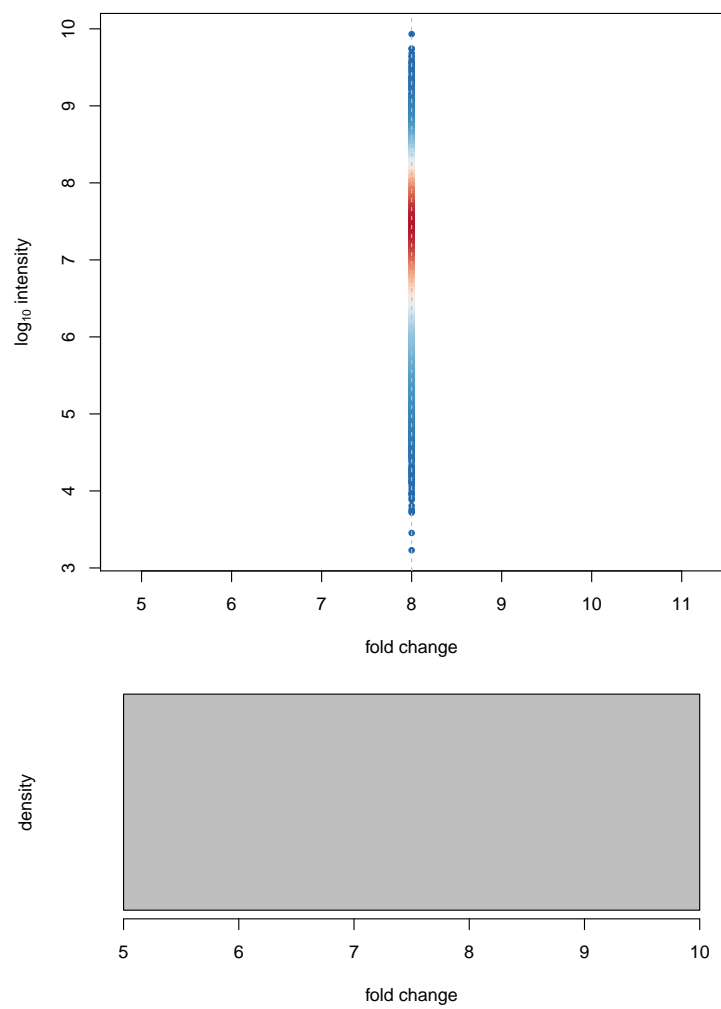


Figure 5: Fold changes of peptide abundances 1 and 2.
 $\text{median}(\text{fc}) = 8$ $\text{sd}(\text{fc}) = 0$

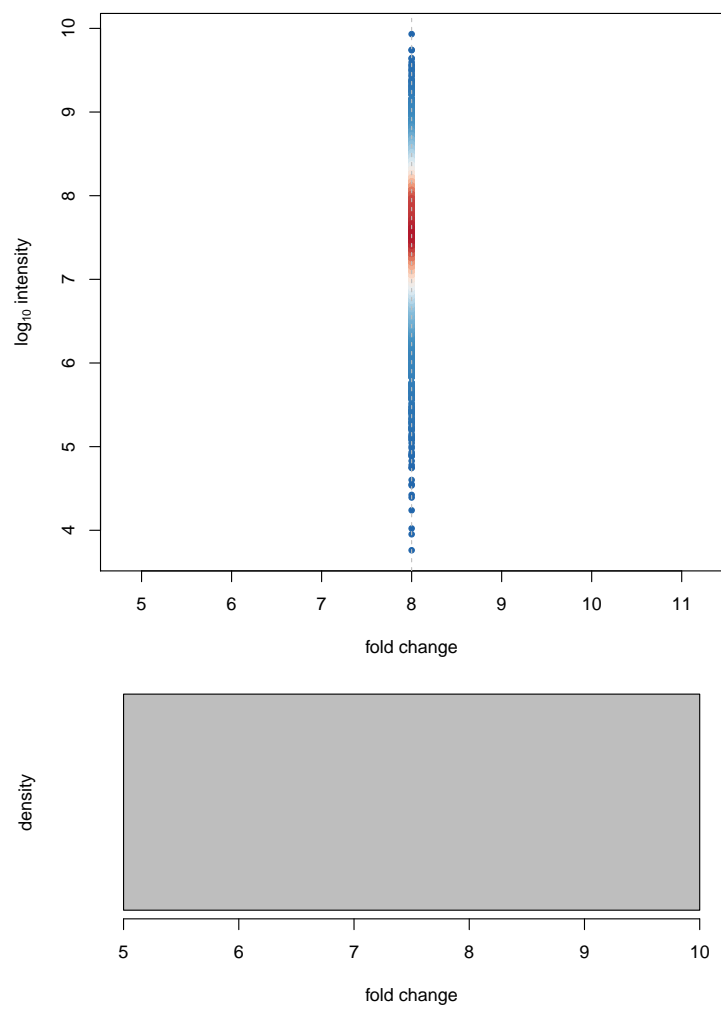


Figure 6: Fold changes of peptide abundances 1 and 3.
 $\text{median}(\text{fc}) = 8$ $\text{sd}(\text{fc}) = 0$

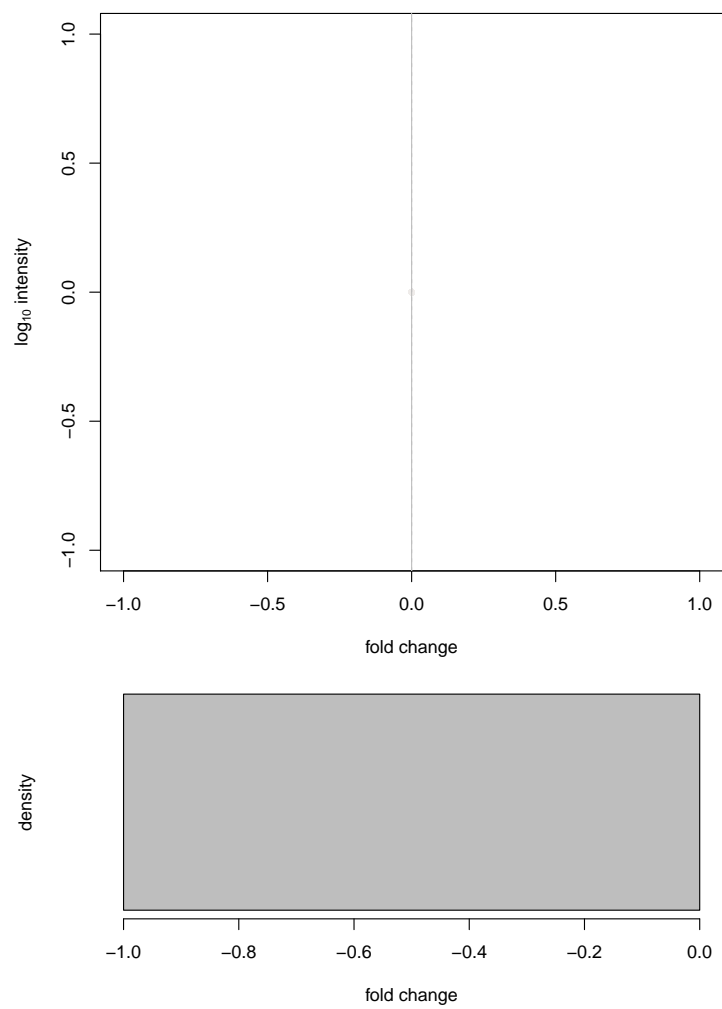


Figure 7: Fold changes of peptide abundances 2 and 3.
 $\text{median}(\text{fc}) = 0$ $\text{sd}(\text{fc}) = 0$

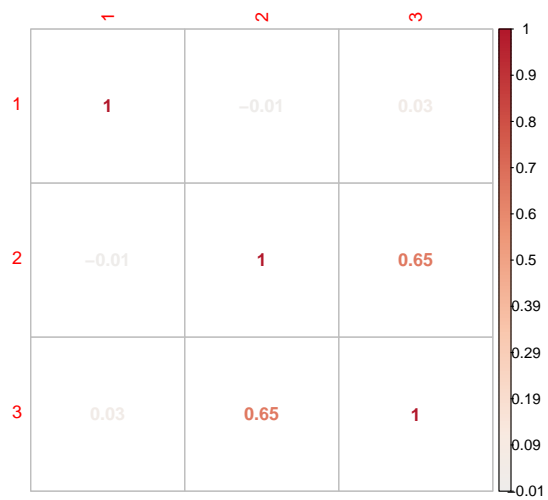


Figure 8: Pearson correlation of all peptide abundances. (min correlation = -0.0099 , median correlation = 0.6539 , max correlation = 1)

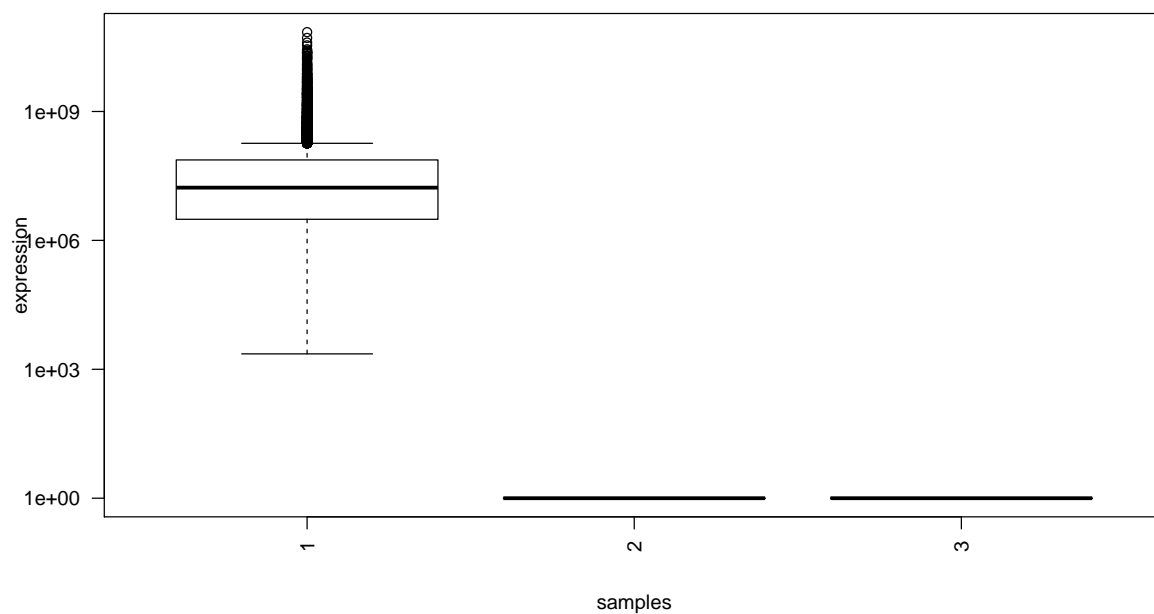


Figure 9: Boxplot of all peptide abundances.

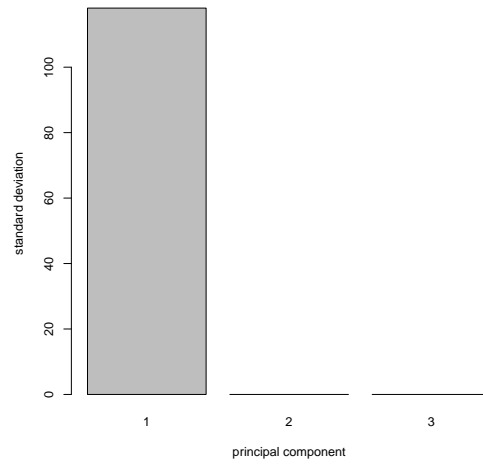


Figure 10: Standard deviation of all principal components.

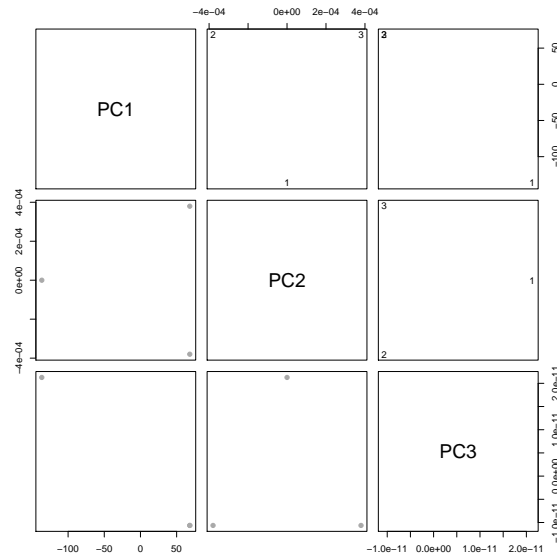


Figure 11: Principal Component Analysis of all peptides with complete quantifications. Any peptides with one or more missing values are ignored. The numbers in the upper right panels correspond to the sample IDs.

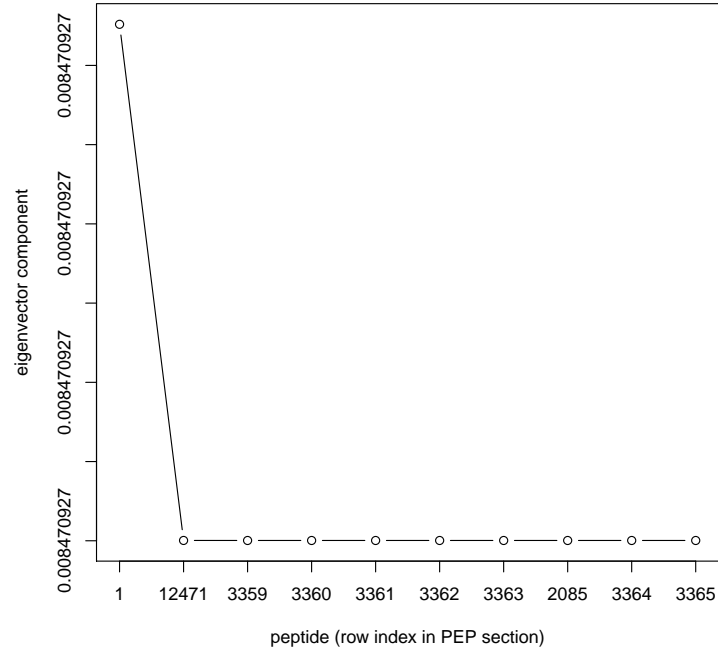


Figure 12: Most important contributions to the first principal component.

| row index | modified sequence | accession | charge | retention time | m/z |
|-----------|-------------------|-----------|--------|----------------|---------|
| 1 | | | 1.00 | 23.01 | 371.32 |
| 12471 | | | 2.00 | 5706.35 | 1075.01 |
| 3359 | | | 3.00 | 2551.71 | 744.71 |
| 3360 | | | 3.00 | 2551.85 | 655.04 |
| 3361 | | | 2.00 | 2552.24 | 462.71 |
| 3362 | | | 2.00 | 2552.25 | 630.34 |
| 3363 | | | 1.00 | 2552.32 | 432.28 |
| 2085 | | | 2.00 | 2172.92 | 784.27 |
| 3364 | | | 2.00 | 2552.60 | 465.27 |
| 3365 | | | 3.00 | 2553.56 | 481.27 |

Table 3: Most important contributions to the first principal component.

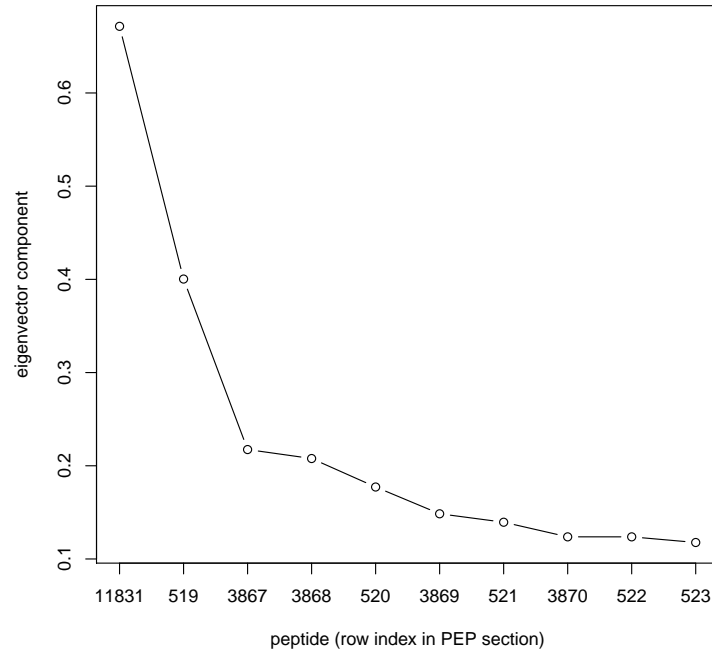


Figure 13: Most important contributions to the second principal component.

| row index | modified sequence | accession | charge | retention time | m/z |
|-----------|-------------------|-----------|--------|----------------|--------|
| 11831 | | | 4.00 | 5444.70 | 614.07 |
| 519 | | | 4.00 | 1518.81 | 486.26 |
| 3867 | | | 3.00 | 2701.36 | 521.30 |
| 3868 | | | 2.00 | 2701.41 | 595.24 |
| 520 | | | 3.00 | 1519.17 | 648.02 |
| 3869 | | | 2.00 | 2701.42 | 542.82 |
| 521 | | | 3.00 | 1520.20 | 537.92 |
| 3870 | | | 2.00 | 2701.56 | 547.34 |
| 522 | | | 3.00 | 1521.64 | 609.59 |
| 523 | | | 3.00 | 1522.29 | 642.61 |

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

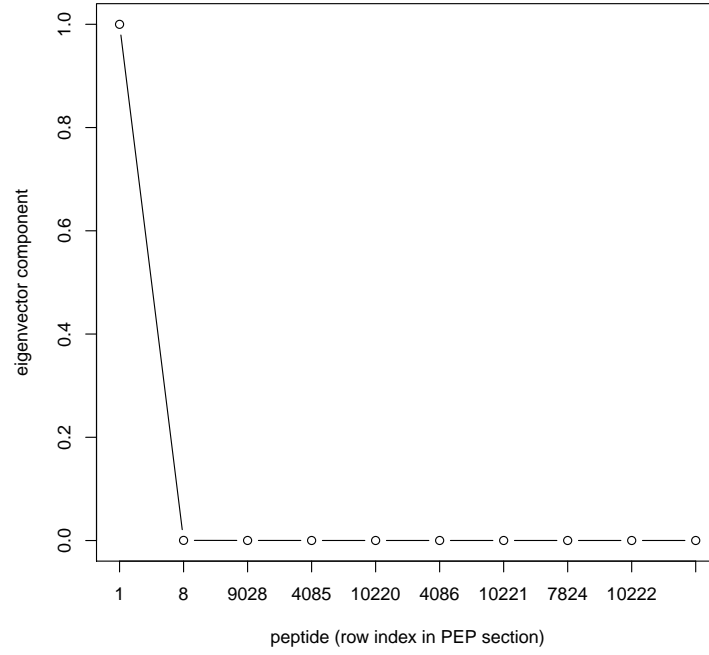


Figure 14: Most important contributions to the third principal component.

| row index | modified sequence | accession | charge | retention time | m/z |
|-----------|-------------------|-----------|--------|----------------|---------|
| 1 | | | 1.00 | 23.01 | 371.32 |
| 8 | | | 1.00 | 189.89 | 428.08 |
| 9028 | | | 2.00 | 4328.71 | 607.34 |
| 4085 | | | 1.00 | 2778.50 | 1054.56 |
| 10220 | | | 2.00 | 4724.57 | 654.83 |
| 4086 | | | 5.00 | 2778.53 | 551.04 |
| 10221 | | | 3.00 | 4724.99 | 553.97 |
| 7824 | | | 2.00 | 3926.45 | 537.80 |
| 10222 | | | 2.00 | 4725.75 | 713.39 |
| 13874 | | | 2.00 | 6403.93 | 747.77 |

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

| 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.