

# Report for PEP Section in mzTab File

## example\_6

The PEP section of the **mzTab** file contains 22,310 quantified peptide features measured in 2 samples.

|                              | number of peptides |        |
|------------------------------|--------------------|--------|
| quantified                   | 22,310             | 100%   |
| quantified (any zero)        | 5,772              | 25.87% |
| quantified (any NaN)         | 0                  | 0%     |
| identified (total)           | 22,310             | 100%   |
| identified (unique modified) | 9,807              | 43.96% |
| identified (unique stripped) | 8,214              | 36.82% |

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.

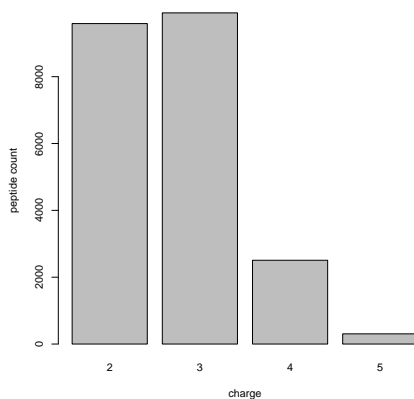


Figure 1: Charge distribution of peptide quantifications.

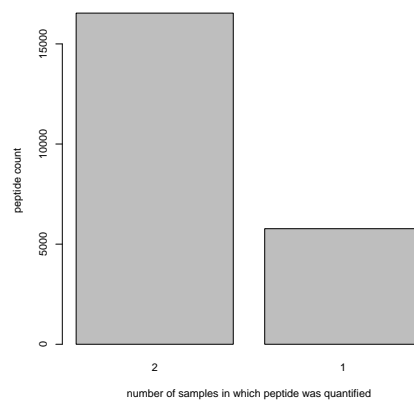


Figure 2: Frequency plot of peptide quantifications.

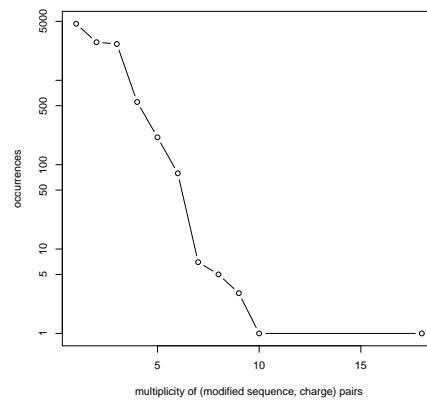


Figure 3: (modified sequence, charge) pair multiplicity vs frequency plot. Each peptide feature (characterised by a (possibly) modified peptide sequence and a charge state) should ideally occur only once in the analysis. In other words, peptides of multiplicity 1 should have a very high frequency. The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

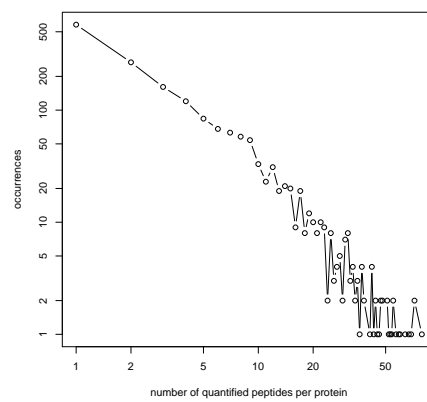


Figure 4: Number of quantified peptides per protein.

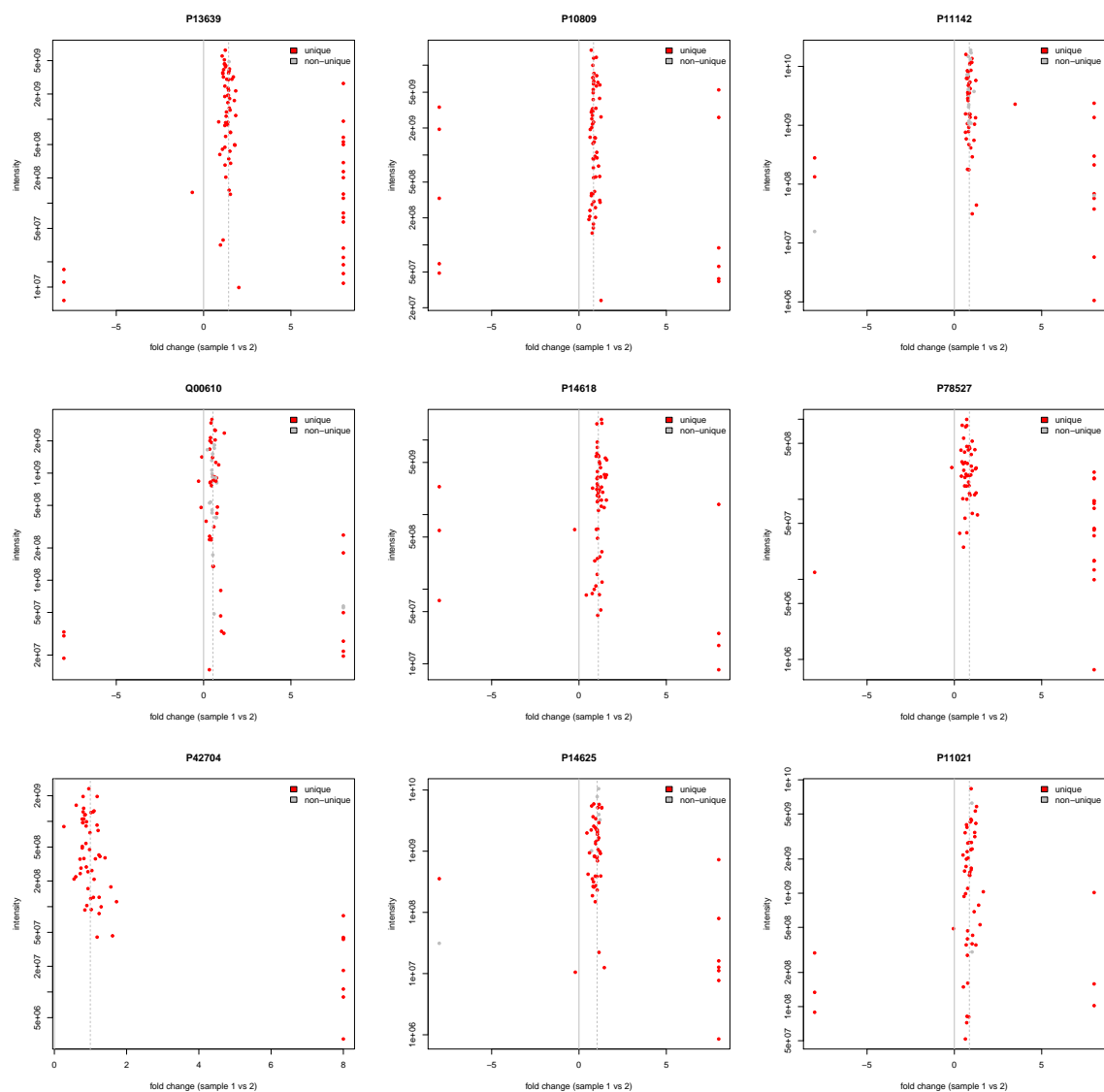
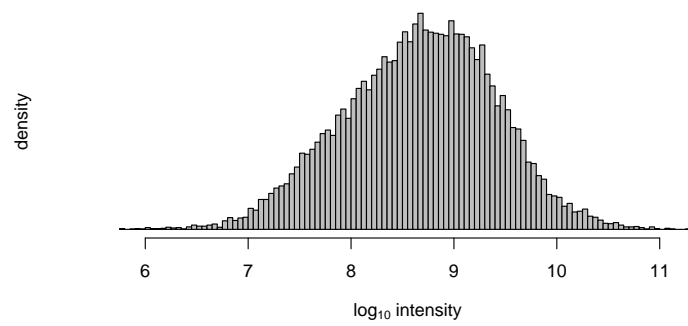
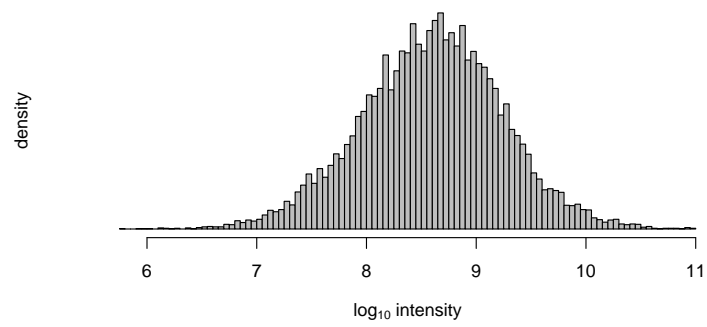


Figure 5: Fold changes of peptide abundances 1 and 2. For proteins with the largest number of quantified peptides.



(a) peptide abundances 1, median(intensity) = 454,615,008



(b) peptide abundances 2, median(intensity) = 243,896,504

Figure 6: peptide abundance distributions.

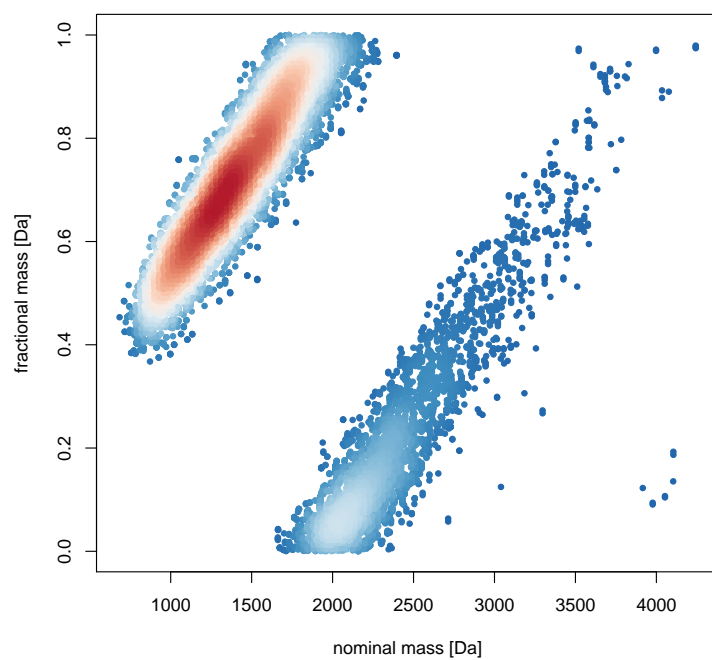


Figure 7: Kendrick nominal fractional mass plot

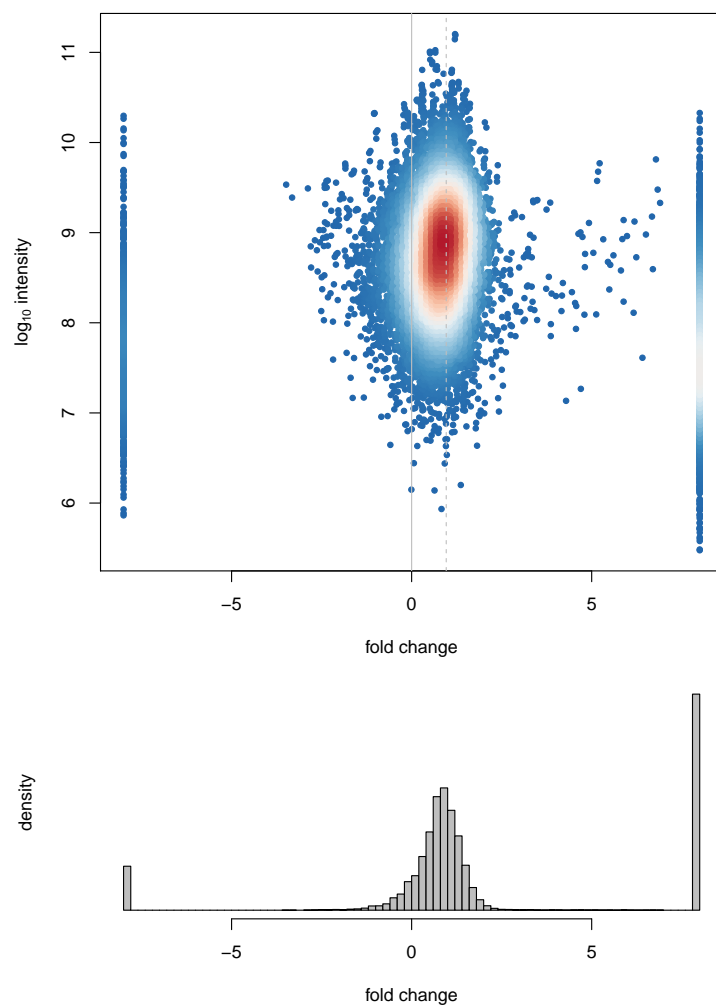


Figure 8: Fold changes of peptide abundances 1 and 2.  
 $\text{median}(fc) = 0.9609$        $\text{sd}(fc) = 3.6836$

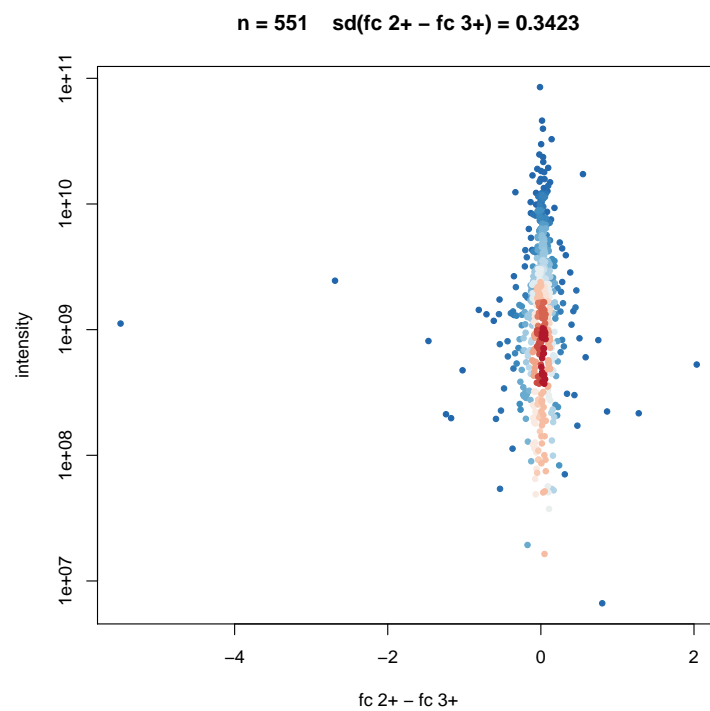


Figure 9: Fold changes of the same peptide in charge 2+ and 3+ are expected to be identical. Here we plot the difference of the 2+ and 3+ fold changes of sample 1 vs. sample 2 of all peptides which were identified and quantified in both charge states.

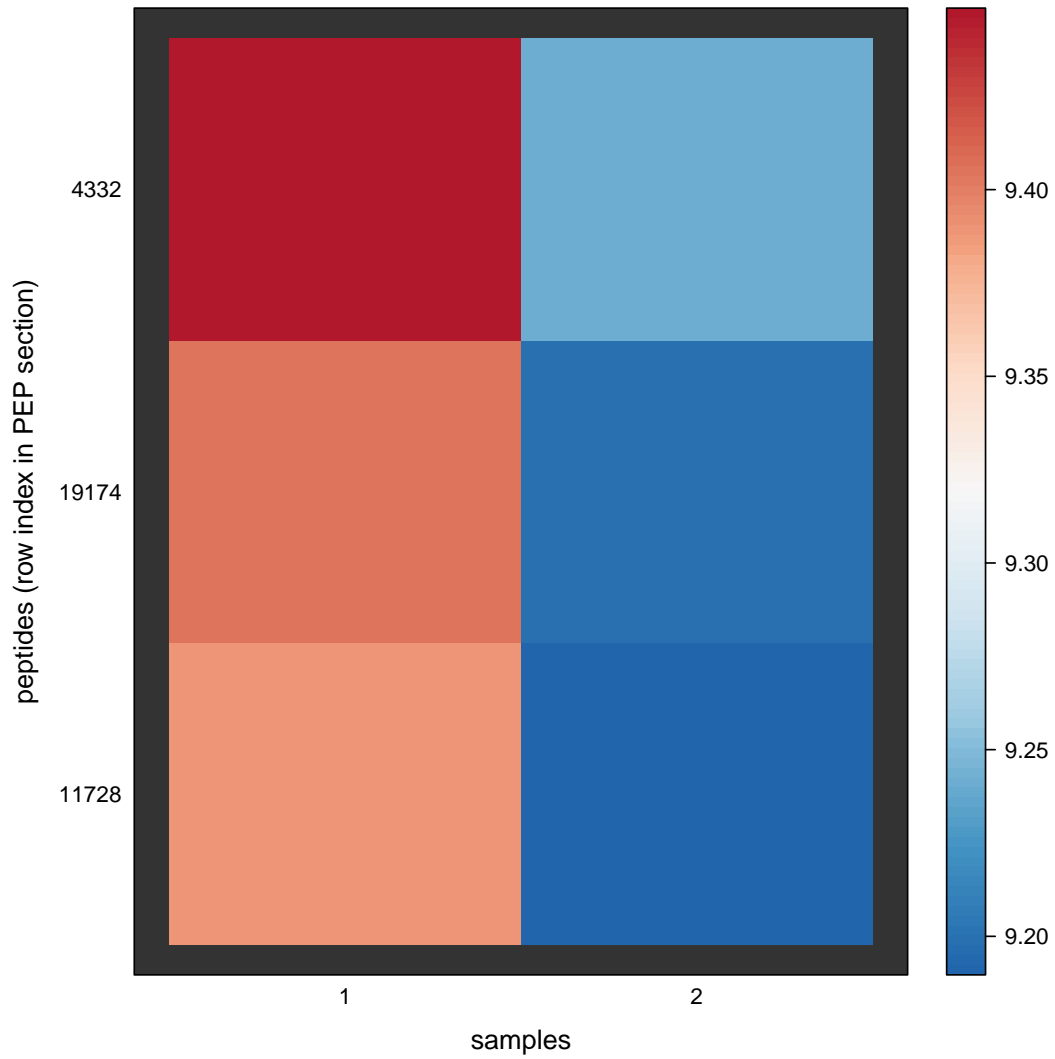


Figure 10: Logarithmic peptide abundances for all peptides of interest.

| row index | modified sequence | accession | charge | retention time | m/z    |
|-----------|-------------------|-----------|--------|----------------|--------|
| 4332      | GILFVGSGVSGGEEGAR | P52209    | 2.00   | 2334.78        | 796.41 |
| 19174     | GILFVGSGVSGGEEGAR | P52209    | 2.00   | 2335.85        | 796.41 |
| 11728     | GILFVGSGVSGGEEGAR | P52209    | 2.00   | 2335.49        | 796.41 |

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.

| row index | modified sequence | accession | charge | retention time | m/z    |
|-----------|-------------------|-----------|--------|----------------|--------|
| 14127     | IAIYELLFK         | P46783    | 2.00   | 3767.59        | 555.33 |
| 6755      | IAIYELLFK         | P46783    | 2.00   | 3772.74        | 555.33 |
| 21653     | IAIYELLFK         | P46783    | 2.00   | 3770.19        | 555.33 |
| 9363      | HPELADKNVPNLHVMK  | P46783    | 4.00   | 1355.06        | 461.25 |
| 2002      | KAEAGAGSATEFQFR   | P46783    | 3.00   | 1385.40        | 523.93 |
| 16849     | KAEAGAGSATEFQFR   | P46783    | 3.00   | 1391.61        | 523.93 |



|       |                              |        |      |         |        |
|-------|------------------------------|--------|------|---------|--------|
| 9428  | KAEAGAGSATEFQFR              | P46783 | 3.00 | 1387.19 | 523.93 |
| 16806 | HPELADKNVPNLHVMK             | P46783 | 4.00 | 1369.56 | 461.25 |
| 1938  | HPELADKNVPNLHVMK             | P46783 | 4.00 | 1356.00 | 461.25 |
| 13450 | DYLHLPPEIVPATLR              | P46783 | 3.00 | 3288.28 | 578.66 |
| 16052 | NVPNLHVMK                    | P46783 | 3.00 | 1030.46 | 351.20 |
| 20332 | DYLHLPPEIVPATLRR             | P46783 | 4.00 | 2891.25 | 473.27 |
| 1999  | KAEAGAGSATEFQFR              | P46783 | 2.00 | 1384.54 | 785.39 |
| 8586  | NVPNLHVMK                    | P46783 | 3.00 | 1021.79 | 351.20 |
| 12851 | DYLHLPPEIVPATLRR             | P46783 | 4.00 | 2888.02 | 473.27 |
| 9422  | KAEAGAGSATEFQFR              | P46783 | 3.00 | 1382.02 | 523.93 |
| 9426  | KAEAGAGSATEFQFR              | P46783 | 2.00 | 1386.17 | 785.39 |
| 16851 | KAEAGAGSATEFQFR              | P46783 | 2.00 | 1392.91 | 785.39 |
| 14761 | GQNLLLTNLQTIQGILER           | P12270 | 3.00 | 4285.16 | 675.39 |
| 22267 | GQNLLLTNLQTIQGILER           | P12270 | 3.00 | 4285.98 | 675.39 |
| 7378  | GQNLLLTNLQTIQGILER           | P12270 | 3.00 | 4293.51 | 675.39 |
| 303   | LSDK(Label:13C(6))VVASVK(... | P12270 | 3.00 | 650.82  | 349.21 |
| 7726  | LSDKVVASVK                   | P12270 | 3.00 | 645.78  | 349.21 |
| 945   | NIEELQQQNQR                  | P12270 | 2.00 | 929.09  | 700.36 |
| 3157  | NLDVQLLDTKR                  | P12270 | 3.00 | 1847.85 | 438.92 |

Table 4: Proteins of interest.

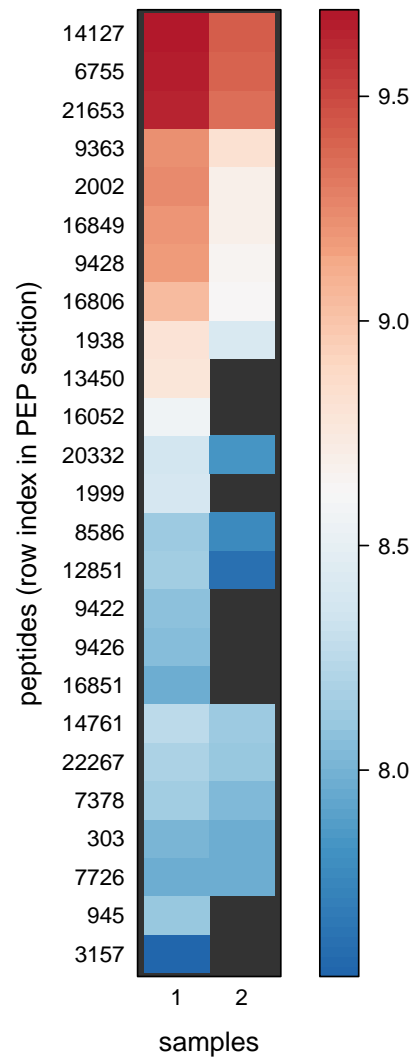


Figure 11: Logarithmic peptide abundances for all proteins of interest.

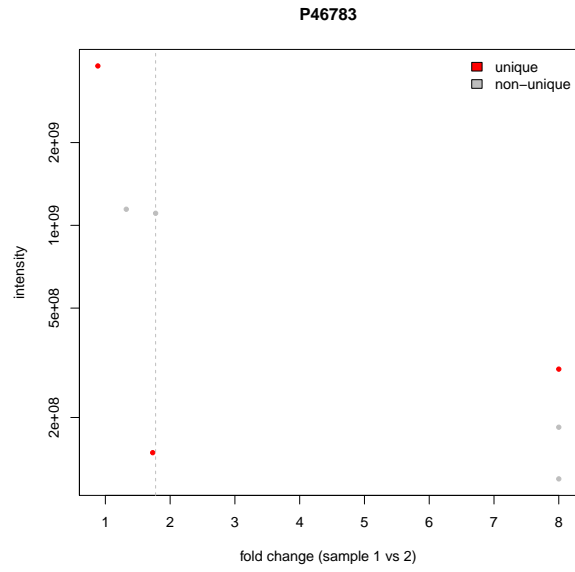


Figure 12: Fold changes of peptide abundances 1 and 2 for first protein of interest.

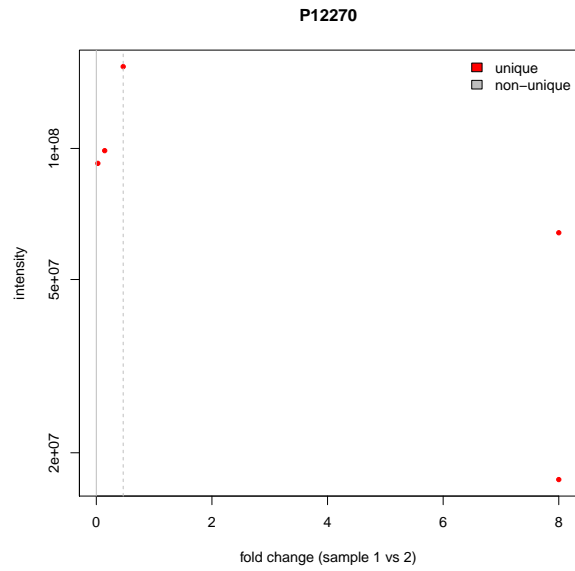


Figure 13: Fold changes of peptide abundances 1 and 2 for second protein of interest.