

Report for PEP Section in mzTab File

example_4

The PEP section of the **mzTab** file contains 1,335 quantified peptide features measured in 54 samples.

| | number of peptides | |
|------------------------------|--------------------|--------|
| quantified | 1,335 | 100% |
| identified (total) | 1,335 | 100% |
| identified (unique modified) | 1,221 | 91.46% |
| identified (unique stripped) | 1,212 | 90.79% |

Table 1: Total number of quantified and identified peptides.

| mod | specificity | number |
|--------------------|-------------|--------|
| Oxidation | M | 179 |
| Methylthio | C | 150 |
| Label:13C(6)15N(2) | K | 6 |
| Label:13C(6)15N(4) | R | 4 |

Table 2: Statistics of modifications.

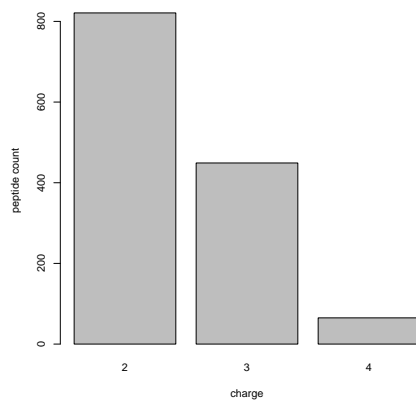


Figure 1: Charge distribution of peptide quantifications.

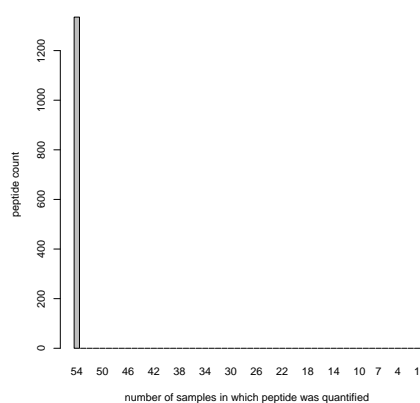


Figure 2: Frequency plot of peptide quantifications.

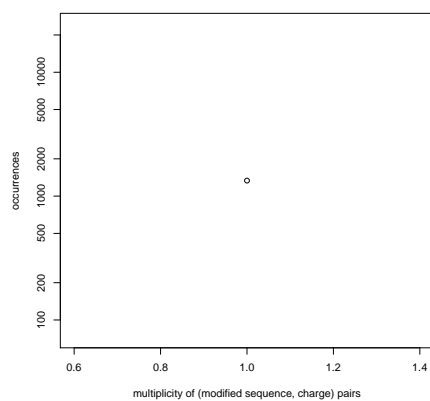


Figure 3: (modified sequence, charge) pair multiplicity vs frequency plot. Each peptide feature (characterised by a (possibly) modified peptide sequence and a charge state) should ideally occur only once in the analysis. In other words, peptides of multiplicity 1 should have a very high frequency. The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

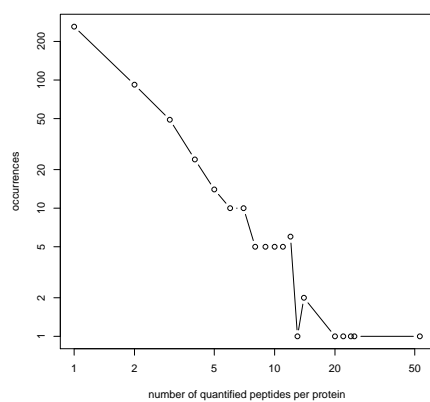


Figure 4: Number of quantified peptides per protein.

| sample | finite | zero | nan |
|--------|--------|------|-----|
| 1 | 1335 | 0 | 0 |
| 2 | 1335 | 0 | 0 |
| 3 | 1335 | 0 | 0 |
| 4 | 1335 | 0 | 0 |
| 5 | 1335 | 0 | 0 |
| 6 | 1335 | 0 | 0 |
| 7 | 1335 | 0 | 0 |
| 8 | 1335 | 0 | 0 |
| 9 | 1335 | 0 | 0 |
| 10 | 1335 | 0 | 0 |
| 11 | 1335 | 0 | 0 |
| 12 | 1335 | 0 | 0 |
| 13 | 1335 | 0 | 0 |
| 14 | 1335 | 0 | 0 |
| 15 | 1335 | 0 | 0 |
| 16 | 1335 | 0 | 0 |
| 17 | 1335 | 0 | 0 |
| 18 | 1335 | 0 | 0 |
| 19 | 1335 | 0 | 0 |
| 20 | 1335 | 0 | 0 |
| 21 | 1335 | 0 | 0 |
| 22 | 1335 | 0 | 0 |
| 23 | 1335 | 0 | 0 |
| 24 | 1335 | 0 | 0 |
| 25 | 1335 | 0 | 0 |
| 26 | 1335 | 0 | 0 |
| 27 | 1335 | 0 | 0 |
| 28 | 1335 | 0 | 0 |
| 29 | 1335 | 0 | 0 |
| 30 | 1335 | 0 | 0 |
| 31 | 1335 | 0 | 0 |
| 32 | 1335 | 0 | 0 |
| 33 | 1335 | 0 | 0 |
| 34 | 1335 | 0 | 0 |
| 35 | 1335 | 0 | 0 |
| 36 | 1335 | 0 | 0 |
| 37 | 1335 | 0 | 0 |
| 38 | 1335 | 0 | 0 |
| 39 | 1335 | 0 | 0 |
| 40 | 1335 | 0 | 0 |
| 41 | 1335 | 0 | 0 |
| 42 | 1335 | 0 | 0 |
| 43 | 1335 | 0 | 0 |
| 44 | 1335 | 0 | 0 |
| 45 | 1335 | 0 | 0 |
| 46 | 1335 | 0 | 0 |
| 47 | 1335 | 0 | 0 |
| 48 | 1335 | 0 | 0 |
| 49 | 1335 | 0 | 0 |
| 50 | 1335 | 0 | 0 |
| 51 | 1335 | 0 | 0 |
| 52 | 1335 | 0 | 0 |
| 53 | 1335 | 0 | 0 |
| 54 | 1335 | 0 | 0 |

Table 3: Statistics of quantifications.

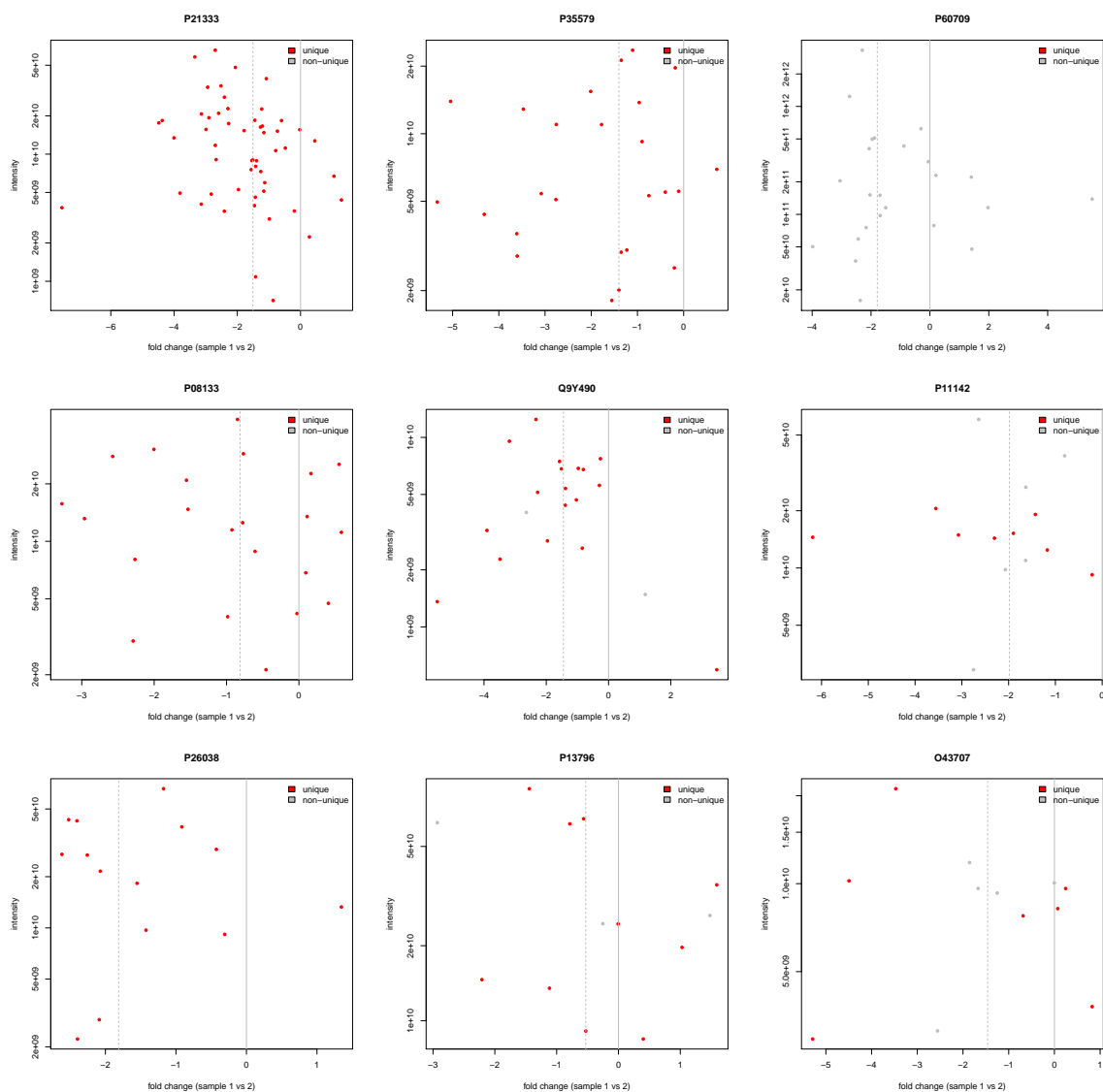
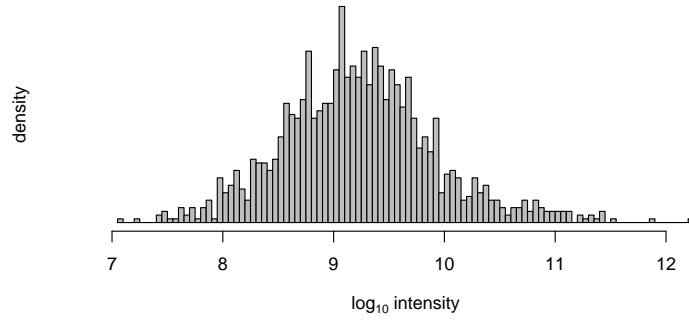
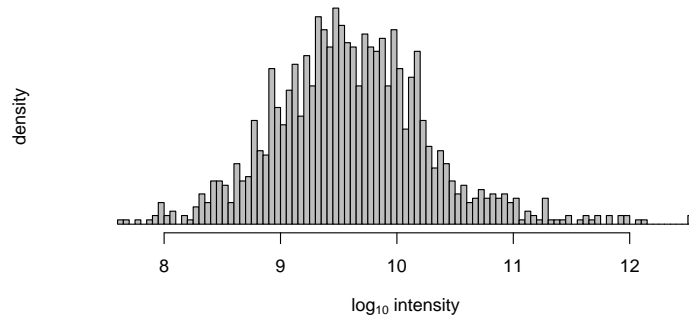


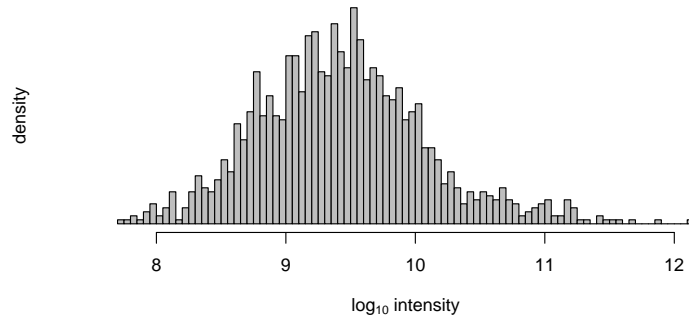
Figure 5: Fold changes of peptide abundances 1 and 2. For proteins with the largest number of quantified peptides.



(a) peptide abundances 1, $\text{median}(\text{intensity}) = 1,605,469,952$



(b) peptide abundances 2, $\text{median}(\text{intensity}) = 3,819,539,968$



(c) peptide abundances 3, $\text{median}(\text{intensity}) = 2,497,959,936$

Figure 6: peptide abundance distributions.

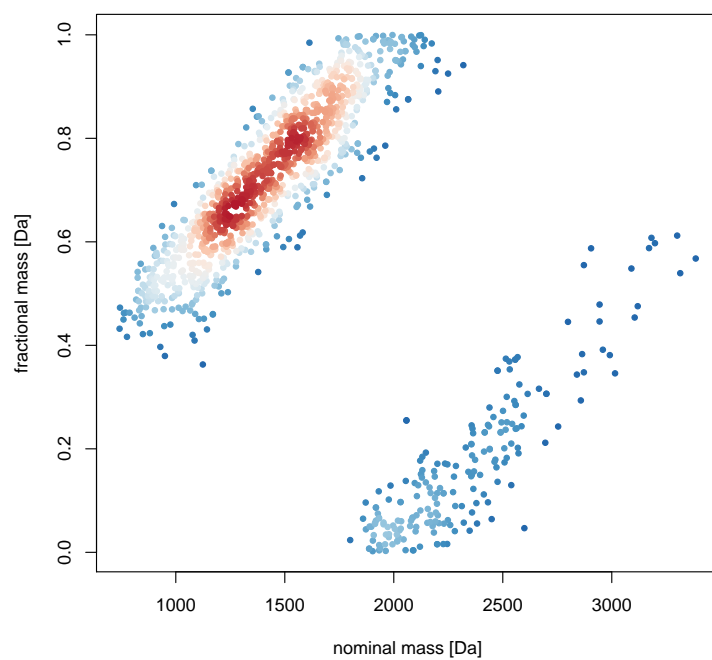


Figure 7: Kendrick nominal fractional mass plot

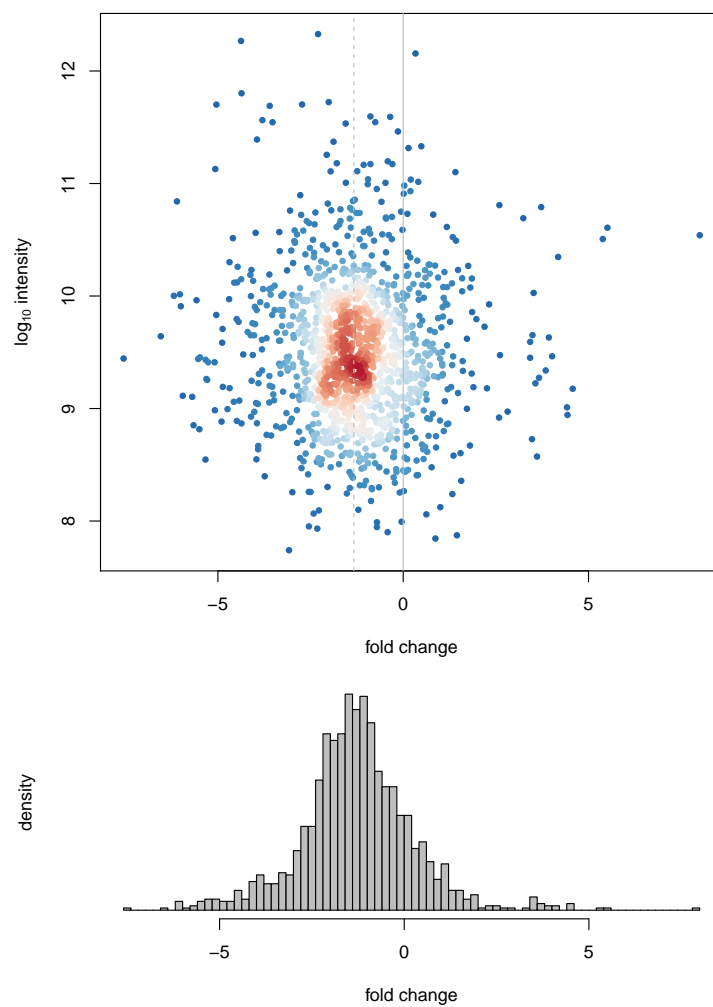


Figure 8: Fold changes of peptide abundances 1 and 2.
 $\text{median}(\text{fc}) = -1.3328$ $\text{sd}(\text{fc}) = 1.5445$

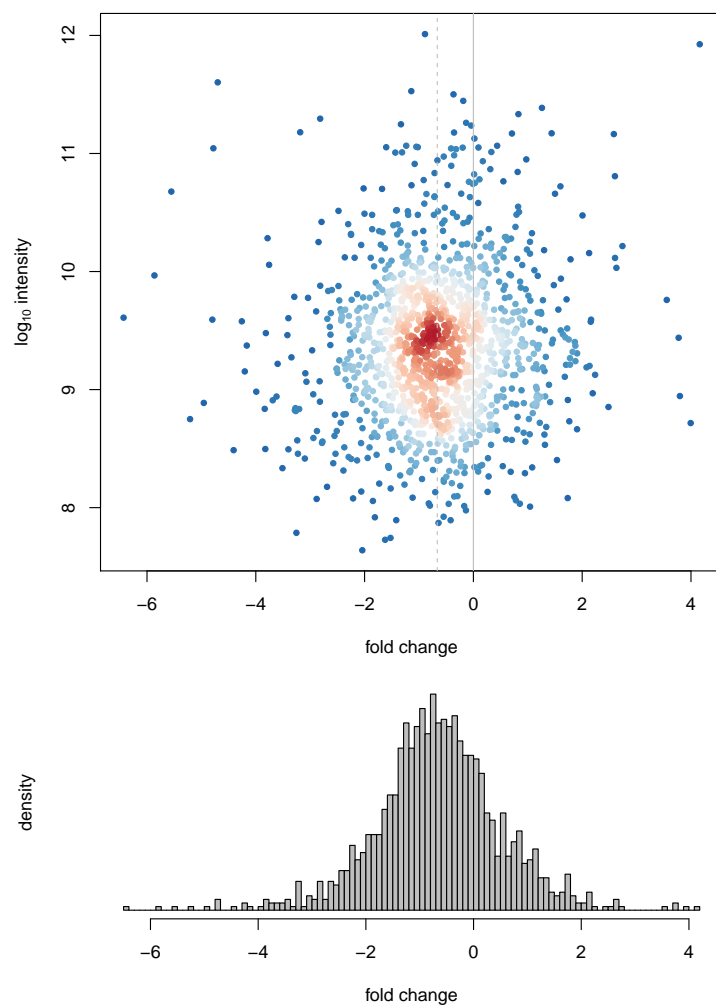


Figure 9: Fold changes of peptide abundances 1 and 3.
 $\text{median}(\text{fc}) = -0.6641$ $\text{sd}(\text{fc}) = 1.1804$

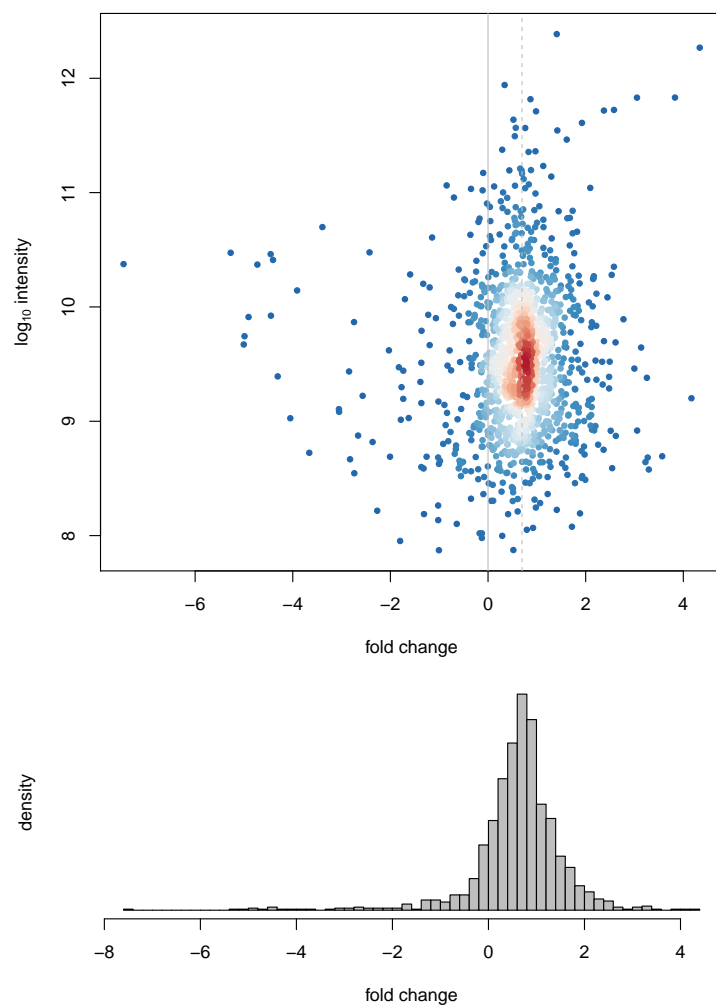


Figure 10: Fold changes of peptide abundances 2 and 3.
 $\text{median}(\text{fc}) = 0.6958$ $\text{sd}(\text{fc}) = 0.9636$

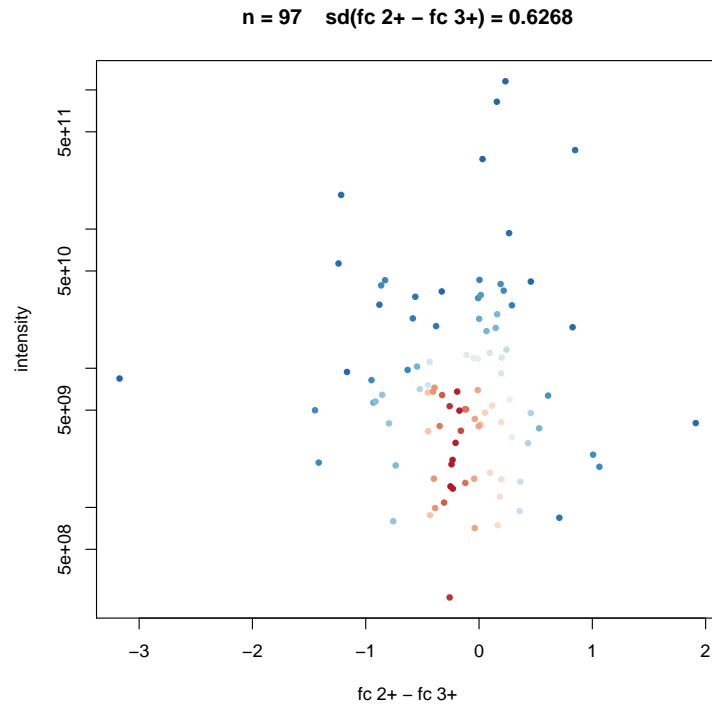


Figure 11: Fold changes of the same peptide in charge 2+ and 3+ are expected to be identical. Here we plot the difference of the 2+ and 3+ fold changes of sample 1 vs. sample 2 of all peptides which were identified and quantified in both charge states.

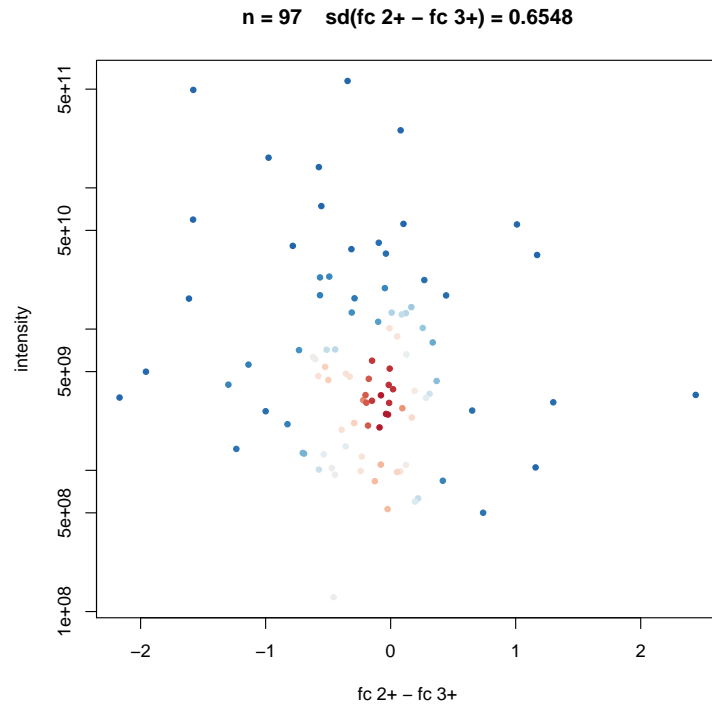


Figure 12: Fold changes of the same peptide in charge 2+ and 3+ are expected to be identical. Here we plot the difference of the 2+ and 3+ fold changes of sample 1 vs. sample 3 of all peptides which were identified and quantified in both charge states.

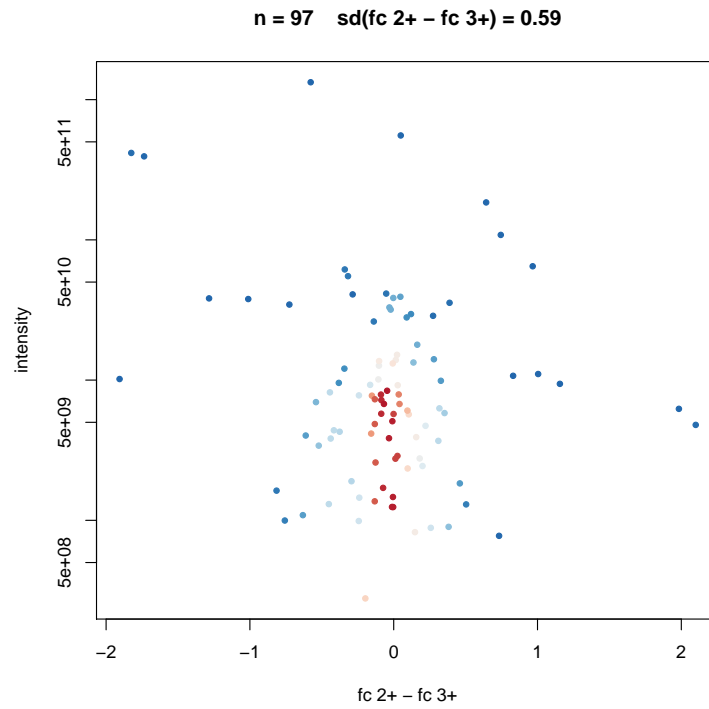


Figure 13: Fold changes of the same peptide in charge 2+ and 3+ are expected to be identical. Here we plot the difference of the 2+ and 3+ fold changes of sample 2 vs. sample 3 of all peptides which were identified and quantified in both charge states.

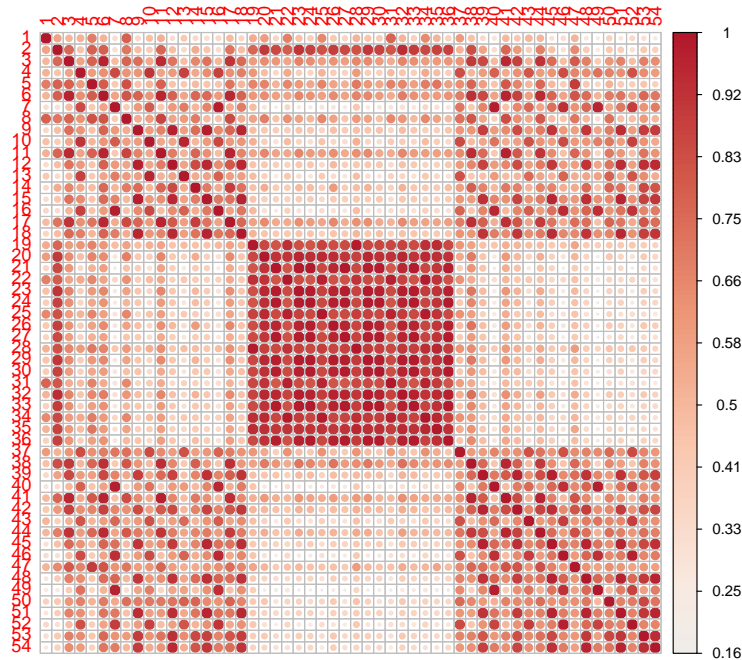


Figure 14: Pearson correlation of all peptide abundances. (min correlation = 0.1622, median correlation = 0.5936, max correlation = 1)

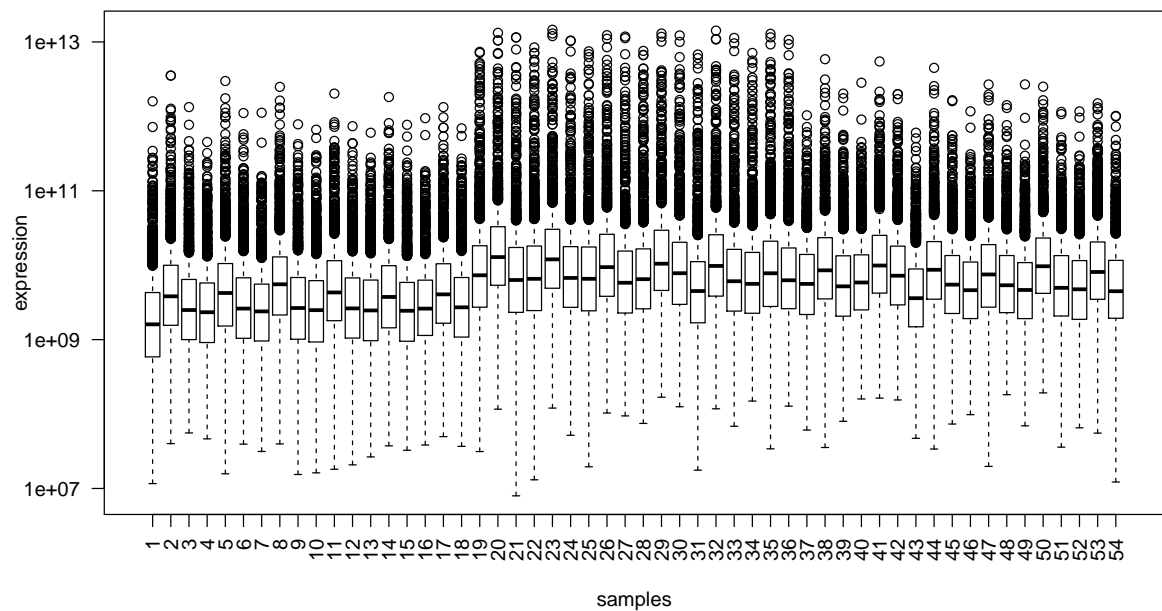


Figure 15: Boxplot of all peptide abundances.

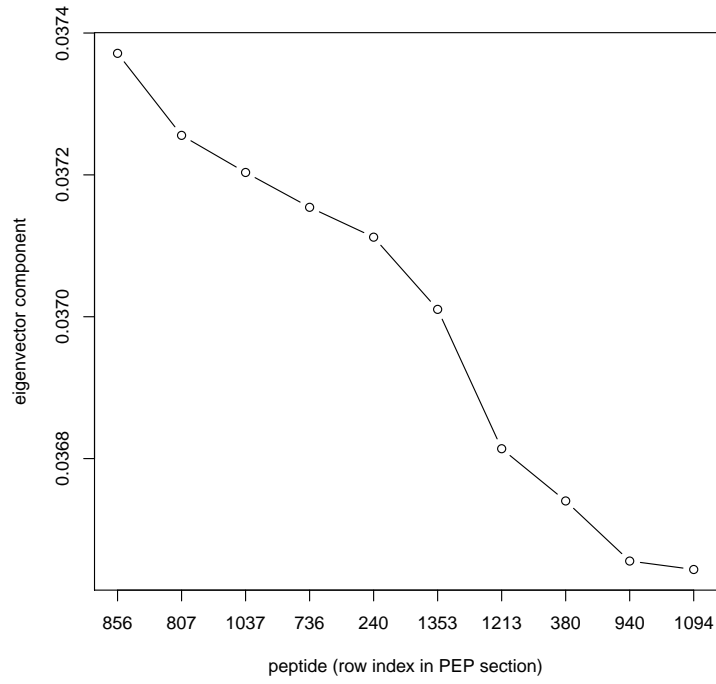


Figure 18: Most important contributions to the first principal component.

| row index | modified sequence | accession | charge | retention time | m/z |
|-----------|------------------------------|-----------|--------|----------------|--------|
| 856 | LVPFDHAESTYGLYR | O95336 | 3 | 6753.43 | 589.96 |
| 807 | TTPPVLDSDGSFFLYSK | P01857 | 2 | 9523.72 | 937.46 |
| 1037 | VLKQVHPDTGISSK | P62807 | 2 | 1911.32 | 754.92 |
| 736 | LYSILGTTLKDEGK | O75083 | 2 | 6063.81 | 769.43 |
| 240 | FLPSELRDEH | Q9Y490 | 2 | 3804.75 | 621.81 |
| 1353 | YGFIEGHVVIPR | P16070 | 3 | 6095.82 | 462.92 |
| 1213 | TPAQYDASELK | P07355 | 2 | 3190.51 | 611.80 |
| 380 | TSASILR | P17987 | 2 | 3663.84 | 430.76 |
| 940 | ILYSQC(Methylthio)GDVM(Ox... | P14649 | 2 | 5333.98 | 673.80 |
| 1094 | ERQEAEAAKEALLQASR | P26038 | 3 | 4365.68 | 653.34 |

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

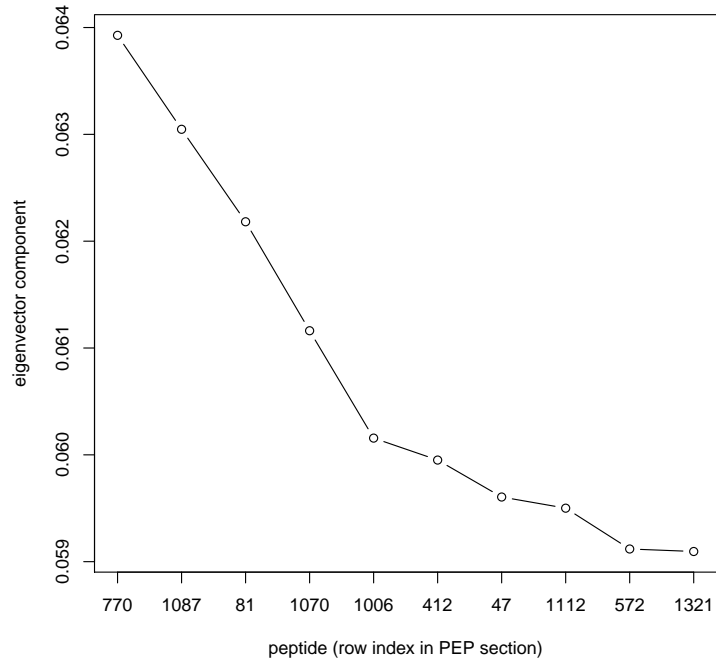


Figure 19: Most important contributions to the second principal component.

| row index | modified sequence | accession | charge | retention time | m/z |
|-----------|--------------------|-----------|--------|----------------|--------|
| 770 | GAVDGGLSIPHSTK | P46777 | 2 | 3445.54 | 669.85 |
| 1087 | AIVAIENPADVSVISSR | P08865 | 2 | 8158.61 | 870.98 |
| 81 | NVHGINFVSPVR | P53634 | 3 | 4626.45 | 446.91 |
| 1070 | SKDIVLVAYSALGSQR | P42330 | 3 | 7358.33 | 569.65 |
| 1006 | IAQSDYIPTQQDVLRL | P04899 | 2 | 6684.21 | 873.95 |
| 412 | LM(Oxidation)VALAK | P07355 | 2 | 3119.97 | 381.23 |
| 47 | LLDAVDITYIPVPLR | P49411 | 2 | 9218.90 | 771.93 |
| 1112 | TPALVNAAVTYSKPR | O75964 | 3 | 4964.94 | 529.97 |
| 572 | IKIGDPLLEDTR | P49189 | 3 | 5956.77 | 457.26 |
| 1321 | SGDSEVYQLGDVSQK | Q04837 | 2 | 5178.78 | 806.38 |

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

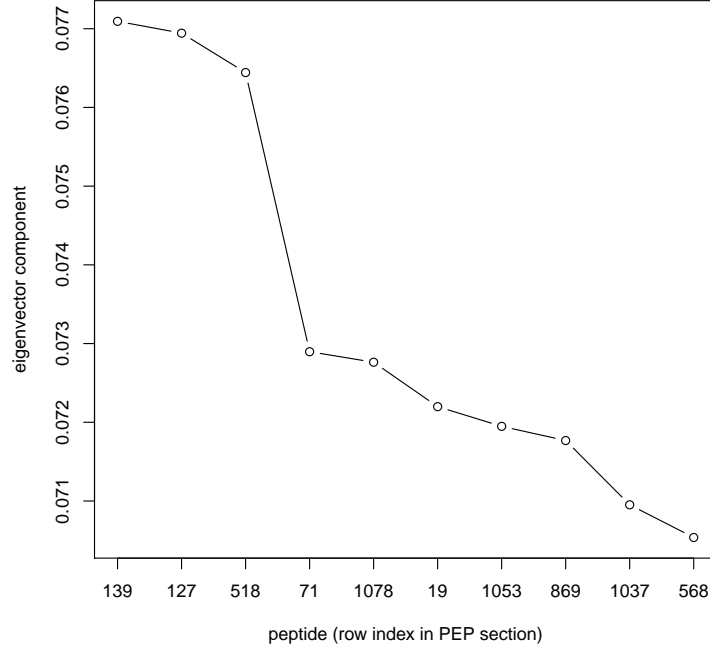


Figure 20: Most important contributions to the third principal component.

| row index | modified sequence | accession | charge | retention time | m/z |
|-----------|----------------------|-----------|--------|----------------|--------|
| 139 | VTAPDVDLHLKAPK | Q09666 | 3 | 4409.15 | 501.96 |
| 127 | KDDLGDITNLHDYLR | Q9NUV9 | 3 | 5318.69 | 558.94 |
| 518 | GFGFVLFK | Q14103 | 2 | 9123.27 | 457.76 |
| 71 | IFVGGLSPDTPEEK | Q14103 | 2 | 6171.10 | 744.88 |
| 1078 | TFVNITPAEVGVLVGKDR | P07737 | 3 | 8764.50 | 639.03 |
| 19 | TIISYIDEQFER | Q15019 | 2 | 9451.35 | 757.38 |
| 1053 | DREVGIPPEQSLETAK | P61158 | 2 | 4599.94 | 884.96 |
| 869 | LAQAAQSSVATITR | Q9Y490 | 2 | 3767.92 | 708.89 |
| 1037 | VLKQVHPDTGISSK | P62807 | 2 | 1911.32 | 754.92 |
| 568 | HIYYITGETKDQVANSFVER | P07900 | 4 | 5448.50 | 611.06 |

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

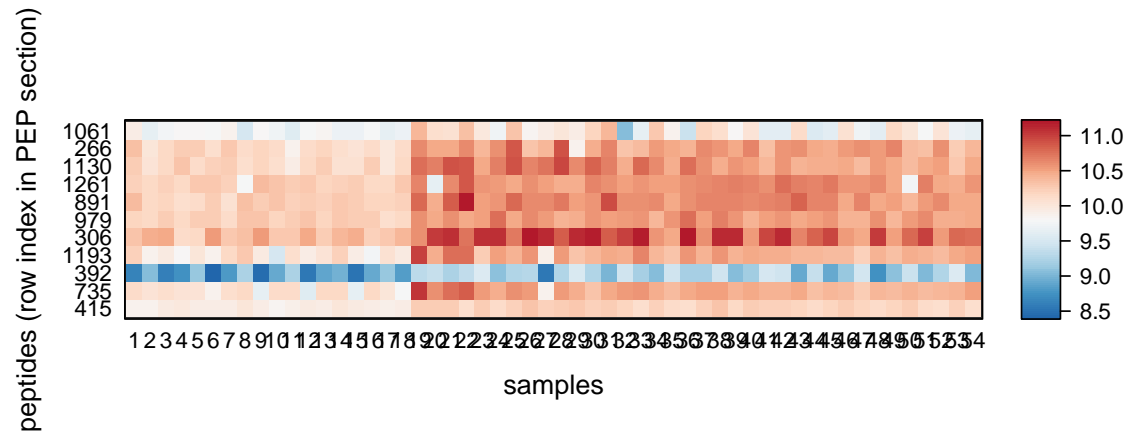


Figure 21: Logarithmic peptide abundances for all peptides of interest.

| row index | modified sequence | accession | charge | retention time | m/z |
|-----------|------------------------------|-----------|--------|----------------|--------|
| 1061 | SSAAPPPPPR(Label:13C(6)15... | STD_01 | 2 | 1659.92 | 493.77 |
| 266 | HVLTSIGEK(Label:13C(6)15N... | STD_03 | 2 | 2127.71 | 496.29 |
| 1130 | IGDYAGIK(Label:13C(6)15N(... | STD_05 | 2 | 3096.71 | 422.74 |
| 1261 | TASEFDSAIAQDK(Label:13C(6... | STD_06 | 2 | 4266.53 | 695.83 |
| 891 | SAAGAFGPESLR(Label:13C(6)... | STD_07 | 2 | 4457.27 | 586.80 |
| 979 | ELGQSGVDTYLQTK(Label:13C(... | STD_08 | 2 | 5741.14 | 773.90 |
| 306 | GLILVGGYGTR(Label:13C(6)1... | STD_09 | 2 | 6431.53 | 558.33 |
| 1193 | GILFVGSGVSGGEEGAR(Label:1... | P52209 | 2 | 6781.34 | 801.41 |
| 392 | GILFVGSGVSGGEEGAR | P52209 | 2 | 6780.92 | 796.41 |
| 735 | SFANQPLEVVYSK(Label:13C(6... | STD_11 | 2 | 6787.30 | 745.39 |
| 415 | ELASGLSFPVGFK(Label:13C(6... | STD_14 | 2 | 9083.08 | 680.37 |

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.

| row index | modified sequence | accession | charge | retention time | m/z |
|-----------|-------------------|-----------|--------|----------------|--------|
| 5 | DYLHLPPEIVPATLRR | P46783 | 3 | 8103.29 | 630.69 |

Table 8: Proteins of interest.

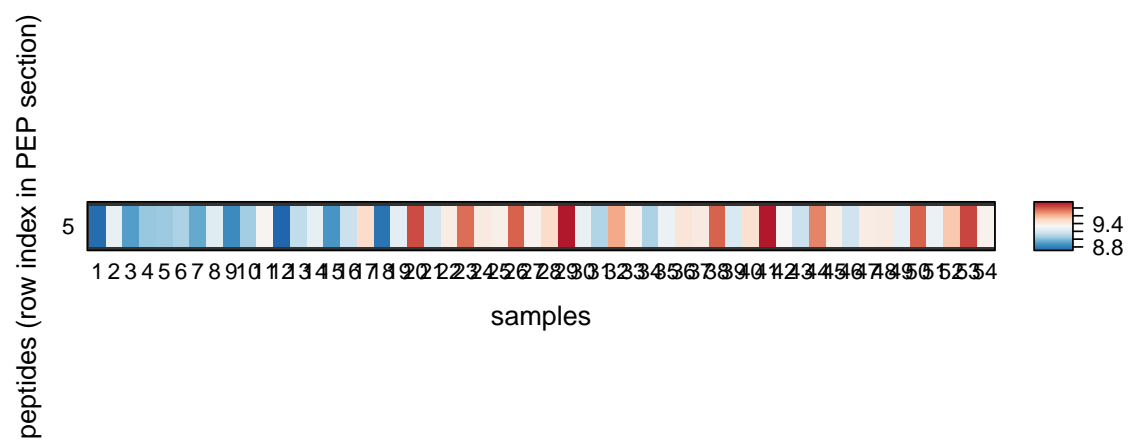


Figure 22: Logarithmic peptide abundances for all proteins of interest.

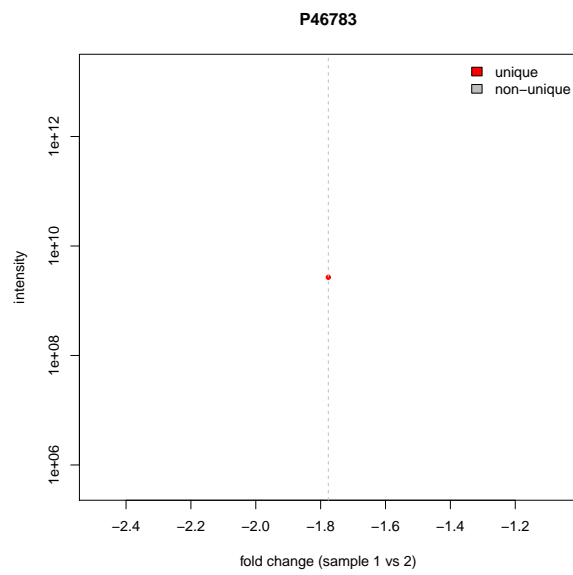


Figure 23: Fold changes of peptide abundances 1 and 2 for first protein of interest.