

Report for PEP Section in mzTab File example_5

The PEP section of the **mzTab** file contains 26,794 quantified peptide features measured in 54 samples.

| | number of peptides |
|------------------------------|--------------------|
| quantified | 26,794 |
| identified (total) | 26,794 |
| identified (unique modified) | 21,658 |
| identified (unique stripped) | 19,580 |

Table 1: Total number of quantified and identified peptides.

| mod | specificity | number |
|--------------------|-------------|--------|
| Oxidation | M | 4942 |
| Methylthio | C | 4473 |
| Dioxidation | M | 112 |
| Label:13C(6)15N(2) | K | 26 |
| Label:13C(6)15N(4) | R | 17 |

Table 2: Statistics of modifications.



Figure 1: Frequency plot of peptide quantifications.

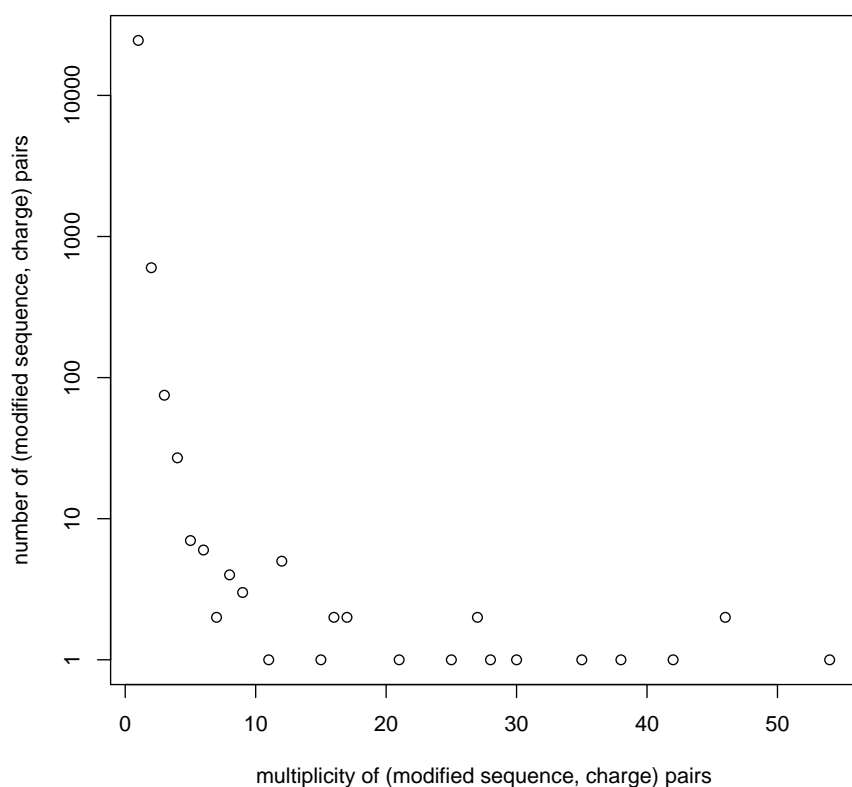
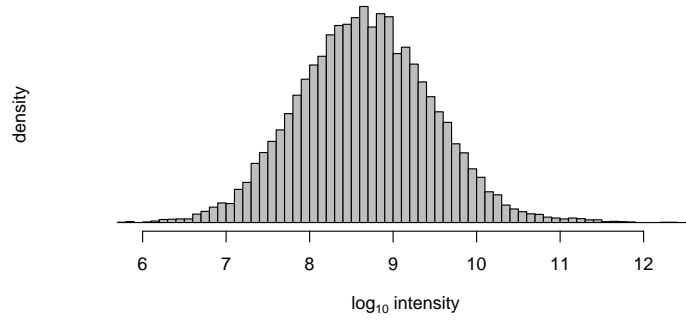


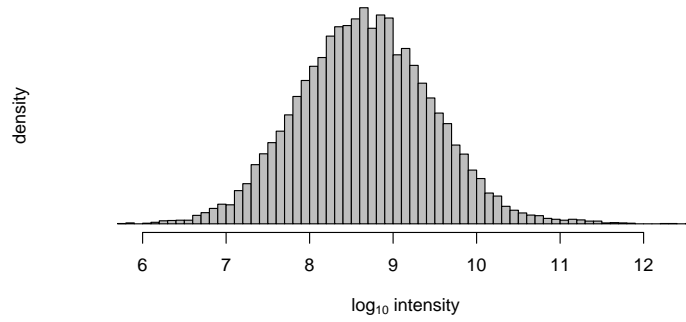
Figure 2: (modified sequence, charge) pair multiplicity vs frequency plot. Each peptide feature (characterised by a (possibly) modified peptide sequence and a charge state) should ideally occur only once in the analysis. In other words, peptides of multiplicity 1 should have a very high frequency. The plot below should show a significant spike on the left and can be used as QC of the analysis.



(a) peptide abundances 1, $\text{median}(\text{intensity}) = 455,025,504$



(b) peptide abundances 2, $\text{median}(\text{intensity}) = 455,025,504$



(c) peptide abundances 3, $\text{median}(\text{intensity}) = 455,025,504$

Figure 3: peptide abundance distributions.

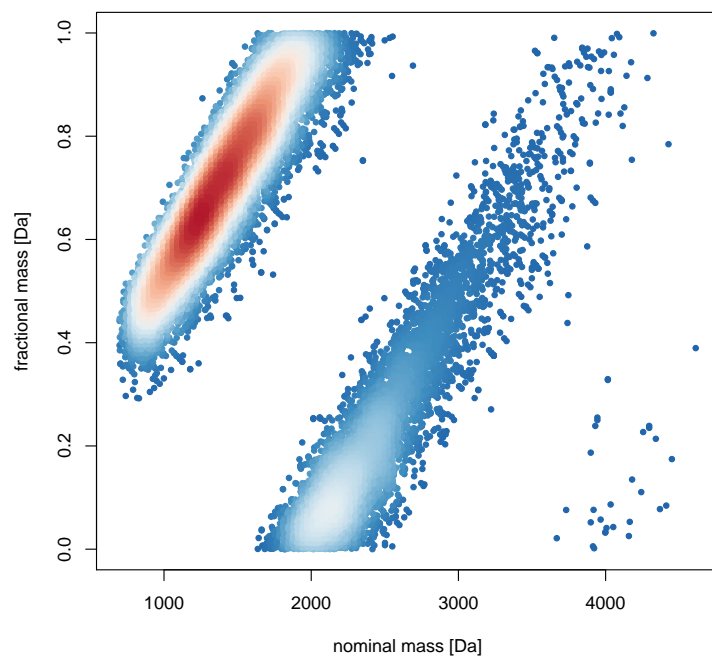


Figure 4: Kendrick nominal fractional mass plot

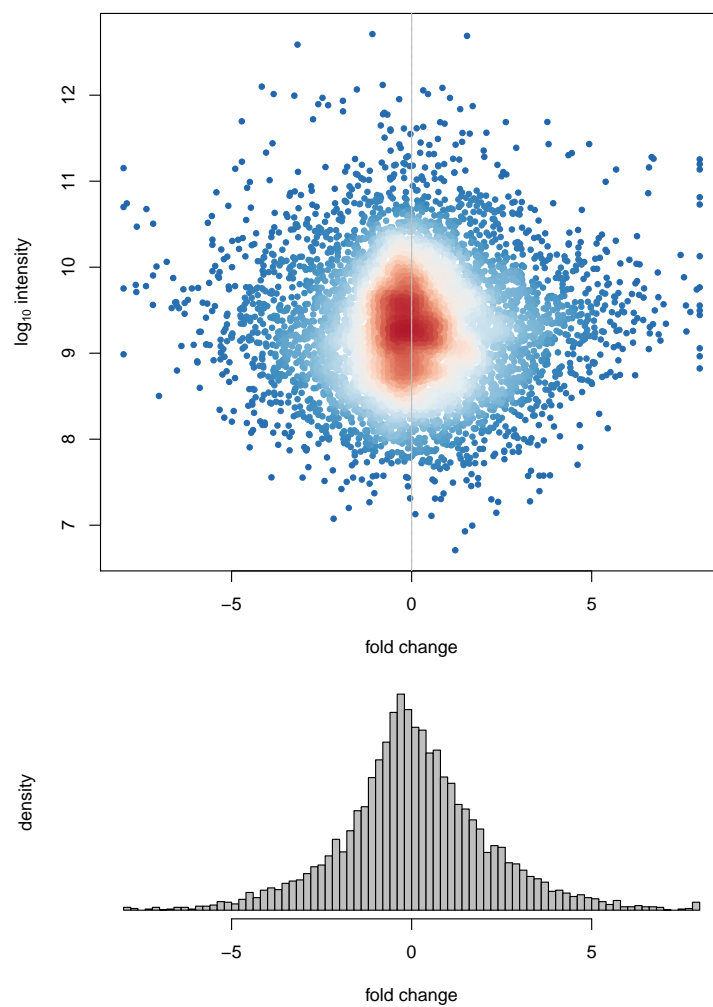


Figure 5: Fold changes of peptide abundances 1 and 2.
 $\text{median}(\text{fc}) = -0.0026$ $\text{sd}(\text{fc}) = 2.0776$

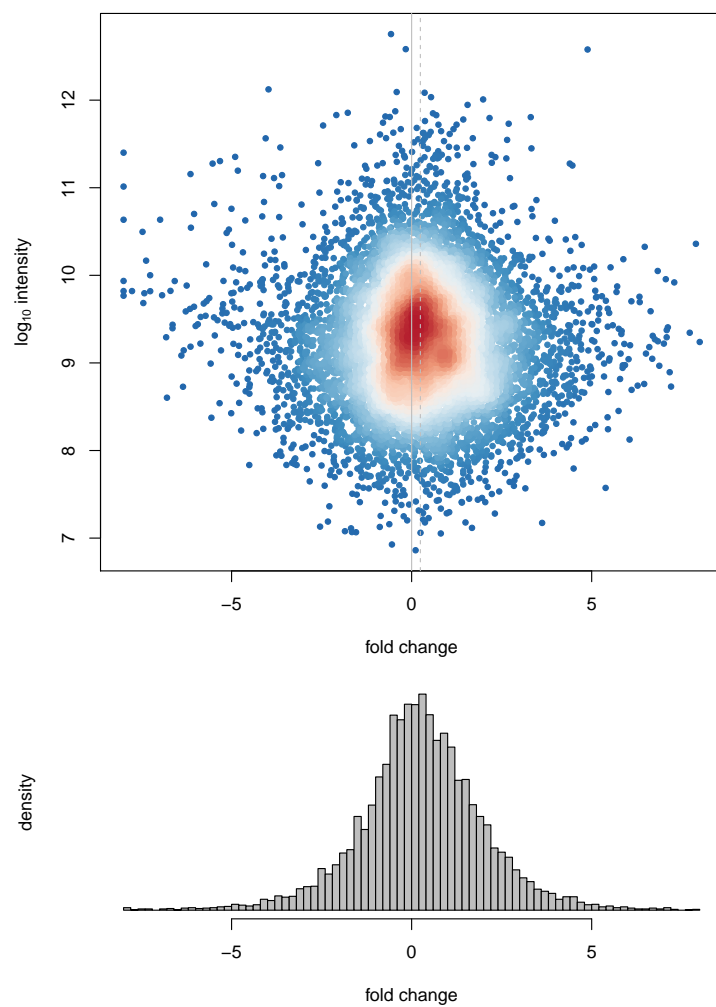


Figure 6: Fold changes of peptide abundances 1 and 3.
 $\text{median}(\text{fc}) = 0.2421$ $\text{sd}(\text{fc}) = 1.7661$

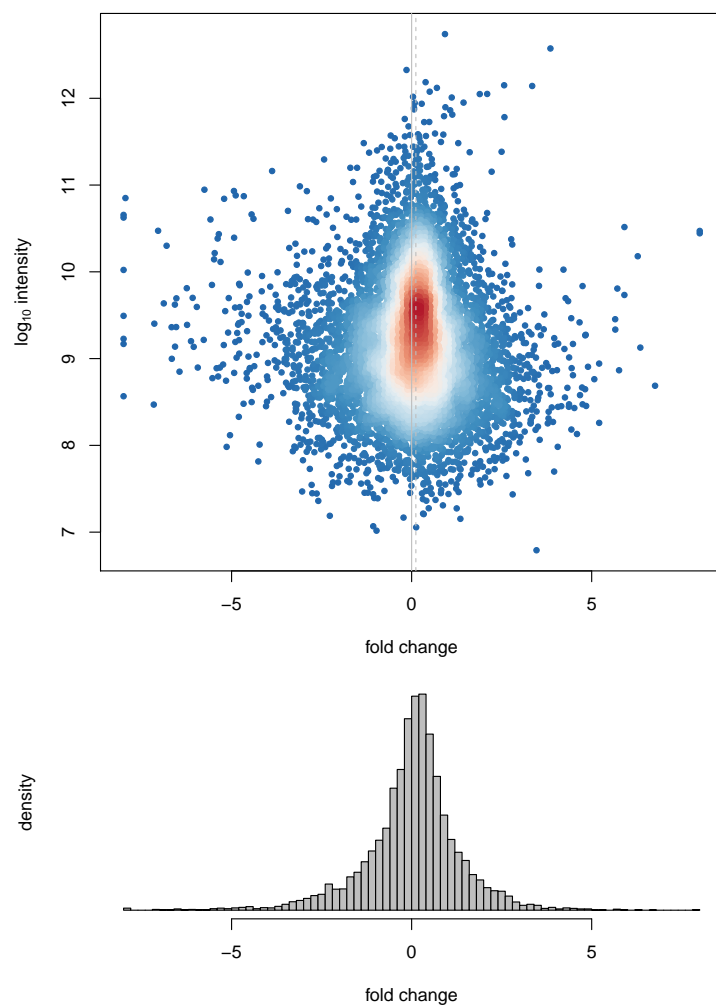


Figure 7: Fold changes of peptide abundances 2 and 3.
 $\text{median}(\text{fc}) = 0.1175$ $\text{sd}(\text{fc}) = 1.3543$

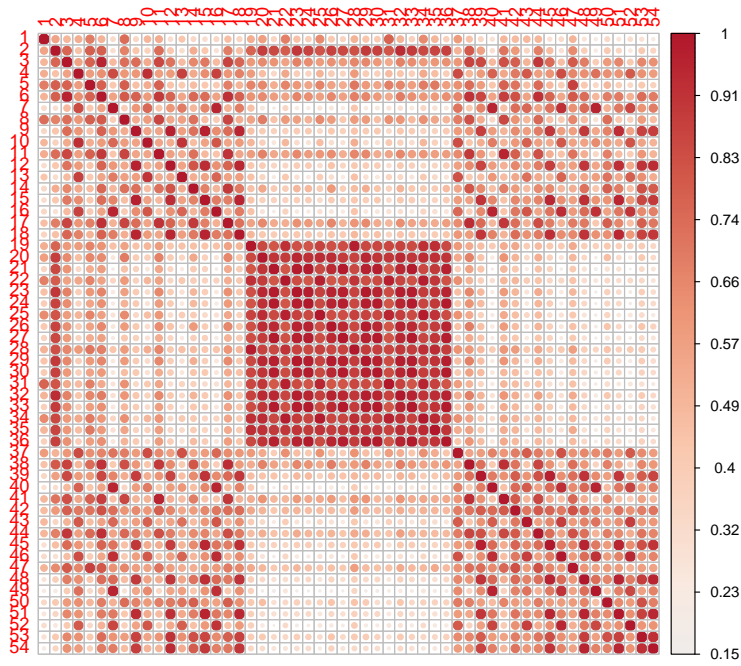


Figure 8: Pearson correlation of all peptide abundances. (min correlation = 0.1484, median correlation = 0.5701, max correlation = 1)

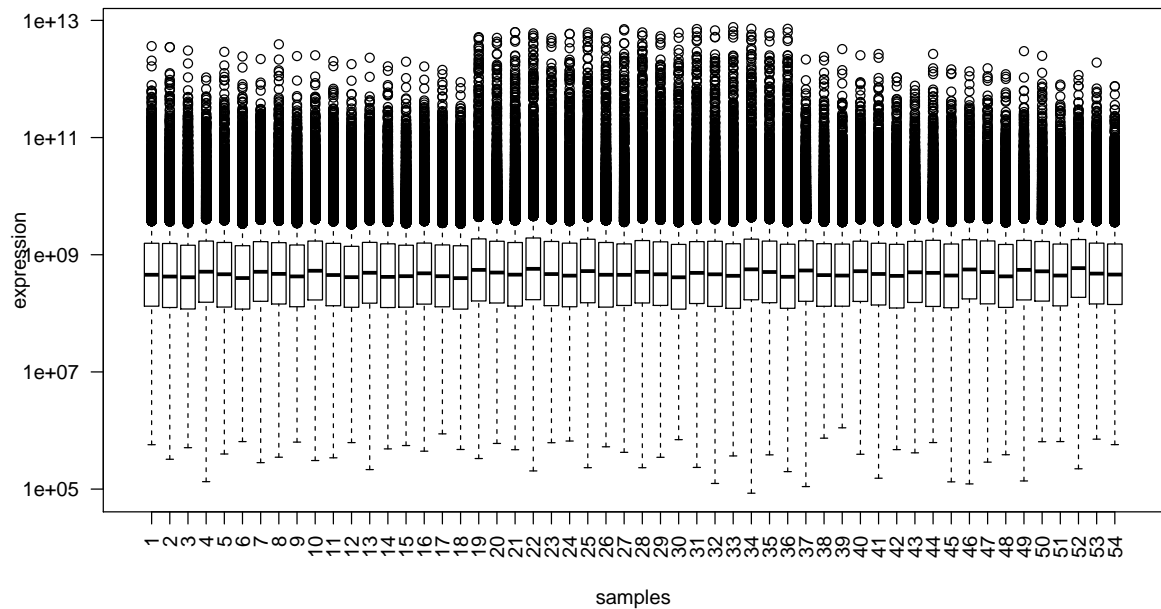


Figure 9: Boxplot of all peptide abundances.

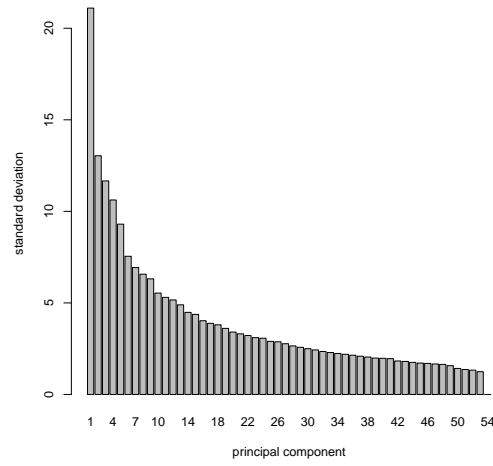


Figure 10: Standard deviation of all principal components.

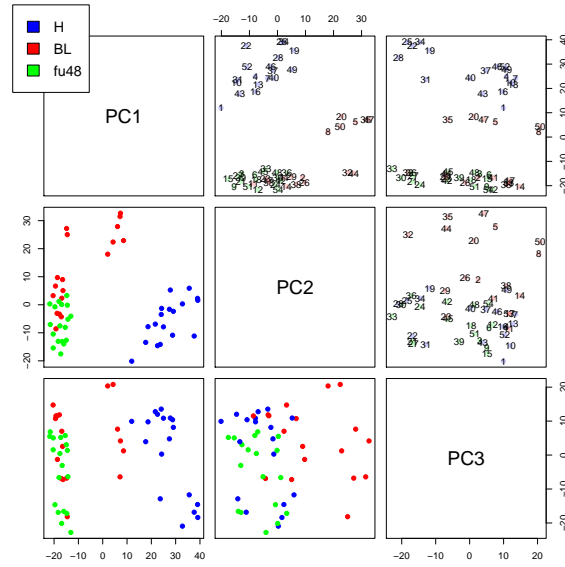


Figure 11: Principal Component Analysis of all peptides with complete quantifications. Any peptides with one or more missing values are ignored. The numbers in the upper right panels correspond to the sample IDs.

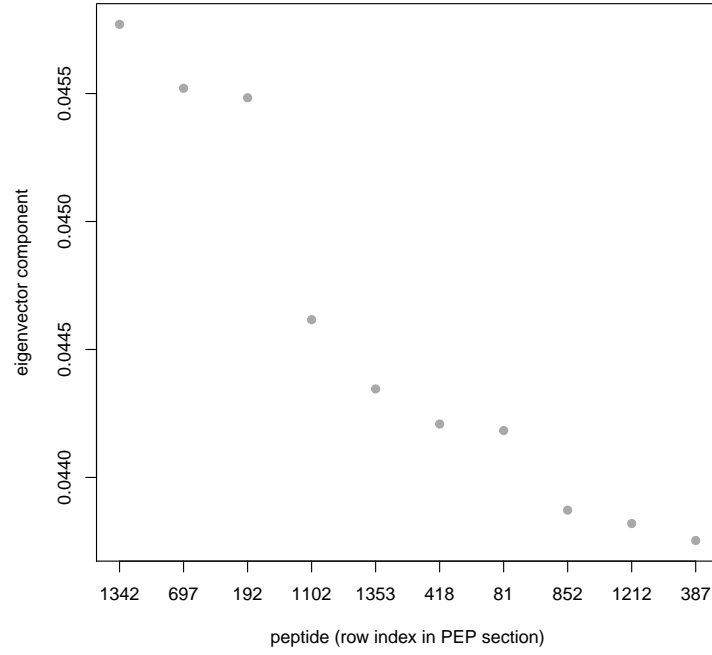


Figure 12: Most important contributions to the first principal component.

| row index | modified sequence | accession | charge | retention time | m/z |
|-----------|------------------------------|-----------|--------|----------------|--------|
| 1342 | IVAPGKGILAADESTGSIK | P04075 | 3 | 5285.58 | 633.36 |
| 697 | YDDM(Oxidation)AAC(Methyl... | P63104 | 2 | 2357.93 | 563.19 |
| 192 | VISGVLQLGNIVFKK | P35579 | 3 | 8817.89 | 539.00 |
| 1102 | NKPLEQSVEDLSKGPPSSVPK | O95466 | 3 | 5083.06 | 746.07 |
| 1353 | IANLQTDLSDGLR | P21333 | 2 | 6841.42 | 708.38 |
| 418 | LIDFLEC(Methylthio)GK | P17844 | 2 | 9345.30 | 542.26 |
| 81 | SAVGFNEM(Oxidation)EAPTTA... | P14317 | 3 | 3498.83 | 620.63 |
| 852 | TIIP LISQC(Methylthio)TPK | P40926 | 2 | 9466.64 | 680.37 |
| 1212 | RTGAIVDVPVGEELLGR | P25705 | 3 | 7675.89 | 594.34 |
| 387 | SETAPAAPAAPAPAEKTPVKK | P10412 | 3 | 2224.46 | 678.04 |

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

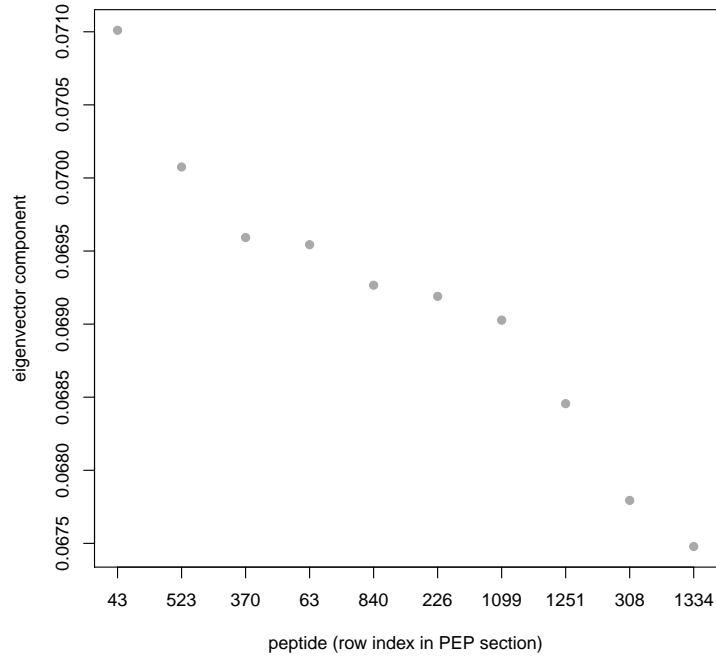


Figure 13: Most important contributions to the second principal component.

| row index | modified sequence | accession | charge | retention time | m/z |
|-----------|------------------------------|-----------|--------|----------------|--------|
| 43 | STPEYFAER | P08133 | 2 | 3515.19 | 550.26 |
| 523 | KQPPVSPGTALVGSQKEPSEVPTPK | P17096 | 3 | 4226.12 | 853.47 |
| 370 | DNHLLGTFDLTGIPPAPR | P11021 | 3 | 9496.78 | 645.34 |
| 63 | DREVGIPPEQSLETAK | P61158 | 3 | 4602.34 | 590.31 |
| 840 | GLPDPALSTQPAPASR | Q14005 | 2 | 5190.93 | 789.42 |
| 226 | LQFHDVAGDIFHQQC(Methylthi... | P11413 | 4 | 7201.68 | 483.73 |
| 1099 | VNLSAAQTLR | Q9BUL8 | 2 | 4025.03 | 536.81 |
| 1251 | ISGASEKDIVHSGLAYTM(Oxidat... | P00367 | 4 | 5040.61 | 545.77 |
| 308 | HVLTSIGEK(Label:13C(6)15N... | STD_03 | 2 | 2127.71 | 496.29 |
| 1334 | HGGTIPIVPTAEFQDR | P00367 | 3 | 6115.00 | 579.97 |

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

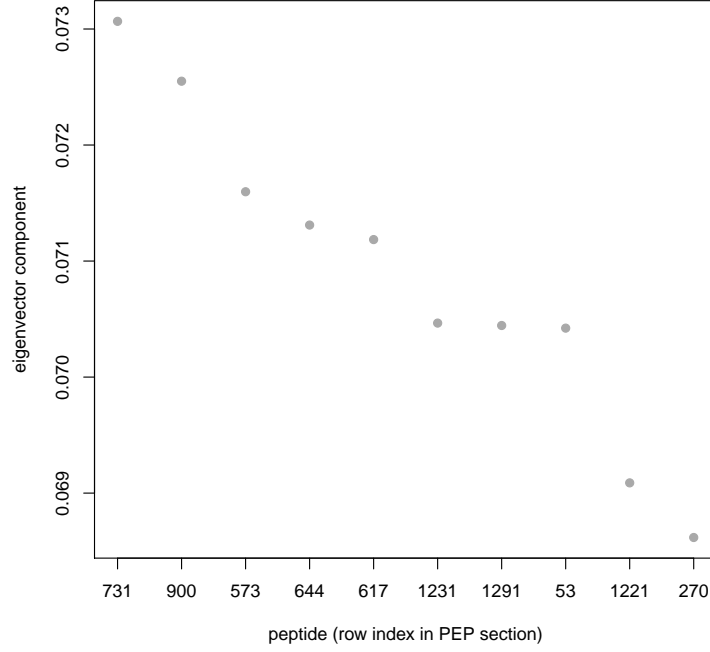


Figure 14: Most important contributions to the third principal component.

| row index | modified sequence | accession | charge | retention time | m/z |
|-----------|------------------------|-----------|--------|----------------|--------|
| 731 | IAFAITAIK | P62269 | 2 | 7044.51 | 474.30 |
| 900 | GITGVEDKESWHGKPLPK | P29401 | 3 | 2940.99 | 660.02 |
| 573 | VALVYGMNEPPGAR | P06576 | 2 | 5752.97 | 801.40 |
| 644 | SSANVEEAFFTLAR | Q92930 | 2 | 9328.50 | 771.38 |
| 617 | SM(Oxidation)YEEEINETR | P20700 | 2 | 3224.81 | 708.80 |
| 1231 | FLIDGFPR | P30085 | 2 | 8094.48 | 482.77 |
| 1291 | AGVAPLQVK | P21333 | 2 | 3134.86 | 441.77 |
| 53 | TETQEKNPLPSKETIEQEK | P62328 | 3 | 2708.84 | 743.71 |
| 1221 | VM(Oxidation)VQPINLIFR | P62304 | 2 | 9095.18 | 673.39 |
| 270 | AVEVQGPSLES GDHGK | Q09666 | 3 | 2851.80 | 537.27 |

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

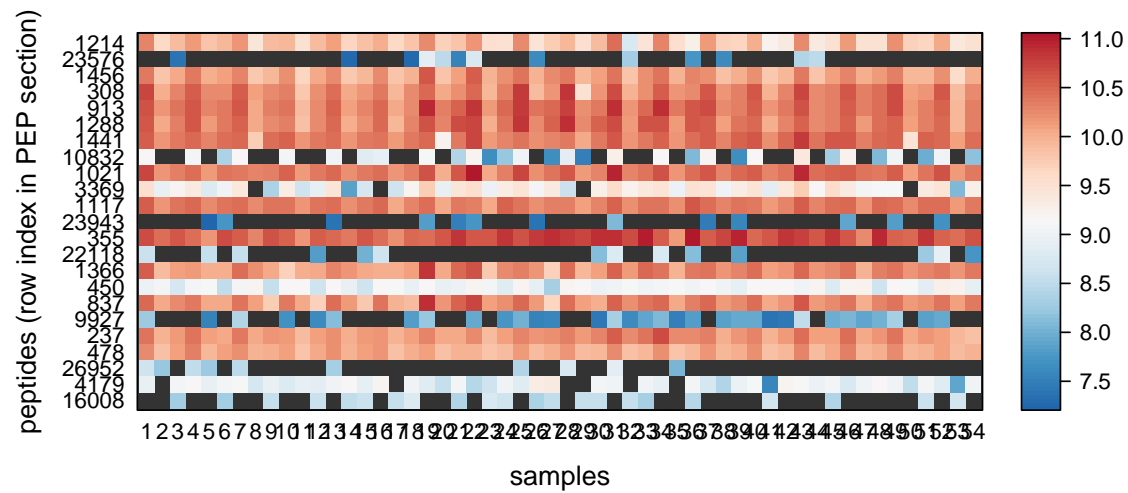


Figure 15: Logarithmic peptide abundances for all peptides of interest.

| row index | modified sequence | accession | charge | retention time | m/z |
|-----------|------------------------------|-----------|--------|----------------|--------|
| 1214 | SSAAPPPPPR(Label:13C(6)15... | STD_01 | 2 | 1659.92 | 493.77 |
| 23576 | SSAAPPPPPR(Label:13C(6)15... | STD_01 | 2 | 1605.04 | 493.76 |
| 1456 | GISNEGQNASIK(Label:13C(6)... | STD_02 | 2 | 2041.39 | 613.32 |
| 308 | HVLTSIGEK(Label:13C(6)15N... | STD_03 | 2 | 2127.71 | 496.29 |
| 913 | DIPVPK(Label:13C(6)15N(2)... | STD_04 | 2 | 2653.71 | 451.28 |
| 1288 | IGDYAGIK(Label:13C(6)15N(... | STD_05 | 2 | 3096.71 | 422.74 |
| 1441 | TASEFDSAIAQDK(Label:13C(6... | STD_06 | 2 | 4266.53 | 695.83 |
| 10832 | TASEFDSAIAQDK | STD_06 | 2 | 4271.48 | 691.83 |
| 1021 | SAAGAFGPESLR(Label:13C(6)... | STD_07 | 2 | 4457.27 | 586.80 |
| 3369 | SAAGAFGPESLR(Label:13C(6)... | STD_07 | 2 | 4650.67 | 586.80 |
| 1117 | ELGQSGVDTYLQTK(Label:13C(... | STD_08 | 2 | 5741.14 | 773.90 |
| 23943 | ELGQSGVDTYLQTK(Label:13C(... | STD_08 | 2 | 5880.07 | 773.90 |
| 355 | GLILVGGYGTR(Label:13C(6)1... | STD_09 | 2 | 6431.53 | 558.33 |
| 22118 | GLILVGGYGTR(Label:13C(6)1... | STD_09 | 2 | 4427.35 | 558.33 |
| 1366 | GILFVGSGVSGGEEGAR(Label:1... | P52209 | 2 | 6781.34 | 801.41 |
| 450 | GILFVGSGVSGGEEGAR | P52209 | 2 | 6780.92 | 796.41 |

| | | | | | |
|-------|------------------------------|--------|---|---------|--------|
| 837 | SFANQPLEVVYSK(Label:13C(6... | STD_11 | 2 | 6787.30 | 745.39 |
| 9927 | SFANQPLEVVYSK(Label:13C(6... | STD_11 | 2 | 6606.62 | 745.39 |
| 237 | LTILEELR(Label:13C(6)15N(... | STD_12 | 2 | 7538.66 | 498.80 |
| 478 | ELASGLSFPVGFK(Label:13C(6... | STD_14 | 2 | 9083.08 | 680.37 |
| 26952 | ELASGLSFPVGFK(Label:13C(6... | STD_14 | 2 | 8764.02 | 680.37 |
| 4179 | LSSEAPALFQFDLK(Label:13C(... | STD_15 | 2 | 9657.05 | 787.42 |
| 16008 | AKGILFVGSGVSGGEEGAR | P52209 | 3 | 4941.74 | 597.65 |

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.

| row index | modified sequence | accession | charge | retention time | m/z |
|-----------|-------------------------------|-----------|--------|----------------|---------|
| 5 | DYLHLPPEIVPATLRR | P46783 | 3 | 8103.29 | 630.69 |
| 1721 | KAEAGAGSATEFQFR | P46783 | 2 | 3516.88 | 785.39 |
| 2475 | AEAGAGSATEFQFR | P46783 | 2 | 5036.50 | 721.34 |
| 2584 | KAEAGAGSATEFQFR | P46783 | 3 | 3518.31 | 523.93 |
| 3119 | IAIYELLFK | P46783 | 2 | 10732.68 | 555.33 |
| 3411 | DYLHLPPEIVPATLRR | P46783 | 4 | 8100.98 | 473.27 |
| 5284 | DYLHLPPEIVPATLR | P46783 | 3 | 9558.62 | 578.66 |
| 8795 | SAVPPGADKKAEAGAGSATEFQFR | P46783 | 4 | 4302.34 | 598.80 |
| 9684 | SAVPPGADKKAEAGAGSATEFQFR | P46783 | 3 | 4302.30 | 798.07 |
| 10741 | GYVKEQFAWR | P46783 | 3 | 4253.53 | 428.56 |
| 11596 | IAIYELLFKEGVM(Oxidation)V... | P46783 | 3 | 10197.44 | 614.01 |
| 15136 | HFYWYLTNEGIQYLR | P46783 | 3 | 9290.39 | 668.33 |
| 15766 | GYVKEQFAWR | P46783 | 2 | 4257.40 | 642.33 |
| 19976 | DYLHLPPEIVPATLR | P46783 | 2 | 9548.91 | 867.48 |
| 20490 | HPELADKNVPSNLHVM(Oxidation... | P46783 | 4 | 2806.75 | 465.25 |
| 25208 | SRPETGRPRPK | P46783 | 2 | 1112.69 | 640.86 |
| 26010 | SRPETGRPRPK | P46783 | 3 | 1112.97 | 427.58 |
| 2595 | LTIHAPPQELGPPVQR | P12270 | 3 | 5244.98 | 585.00 |
| 4982 | NLQEQTVQLQSELSR | P12270 | 2 | 6830.64 | 886.96 |
| 5219 | TLSSVQNEVQEALQR | P12270 | 2 | 7739.83 | 851.44 |
| 5886 | ISTQLDFASK | P12270 | 2 | 4987.08 | 555.30 |
| 11076 | LSQELEYLTEDVKR | P12270 | 3 | 6542.97 | 574.97 |
| 11273 | GIASDPPPTANIKPTPVVSTPSK | P12270 | 3 | 4902.51 | 789.09 |
| 11949 | FKVESEQQYFEIEKR | P12270 | 3 | 4954.28 | 654.00 |
| 13013 | RPSTSQTVSTPAPVPVIESTEAEIA... | P12270 | 3 | 6727.12 | 899.14 |
| 13171 | LENEVEQR | P12270 | 2 | 1693.68 | 508.75 |
| 13646 | LESALTELEQLRK | P12270 | 3 | 6908.25 | 510.62 |
| 13673 | YLDEIVKEVEAK | P12270 | 3 | 7196.92 | 479.26 |
| 14084 | LSSQIEKLEHEISHLK | P12270 | 4 | 6322.55 | 473.51 |
| 14534 | GQNLLLTNLQTIQGILER | P12270 | 2 | 12445.40 | 1012.58 |
| 14775 | NLDVQLLDTK | P12270 | 2 | 6805.16 | 579.82 |
| 15566 | LLSEKEVHTK | P12270 | 2 | 1506.47 | 592.33 |
| 15882 | EKEIAETRFEVAQVESLR | P12270 | 3 | 5813.97 | 712.04 |
| 17342 | ILLSQTTGVAIPLHASSLDDVSLAS... | P12270 | 3 | 9456.43 | 945.52 |
| 18730 | FLADQQSEIDGLKGRHEK | P12270 | 4 | 3196.05 | 518.52 |
| 20518 | KLELDILPLQEANAELSEK | P12270 | 3 | 9473.26 | 718.40 |
| 22013 | EKGNEILELK | P12270 | 2 | 3452.76 | 586.83 |
| 22088 | LQEQVTDLR | P12270 | 2 | 3580.96 | 551.30 |
| 23121 | TKEELEAEKR | P12270 | 2 | 1216.40 | 616.83 |
| 23610 | EGVQGPNVSLSEEGKSQEQILEIL... | P12270 | 3 | 10181.28 | 951.51 |
| 24602 | SAADDSEAKSNELTR | P12270 | 3 | 1865.12 | 531.92 |
| 25260 | ITELQLKLESALTELEQLRK | P12270 | 4 | 10747.62 | 589.59 |
| 26016 | AALKQLQEIFYENYKK | P12270 | 4 | 6949.96 | 456.51 |

| | | | | | |
|-------|---------------------------|--------|---|---------|---------|
| 26106 | SSEQILEILR | P12270 | 2 | 7860.87 | 614.85 |
| 26244 | AADSQNSGEGNTGAAESSFSQEVSR | P12270 | 2 | 4519.04 | 1243.53 |
| 26421 | SAADDSEAKSNELTR | P12270 | 2 | 1834.45 | 797.37 |
| 26635 | KLENEVEQR | P12270 | 2 | 1635.88 | 572.80 |

Table 7: Proteins of interest.

