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%
quantified (any zero)	0	0%
quantified (any NaN)	0	0%
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. (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.

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.

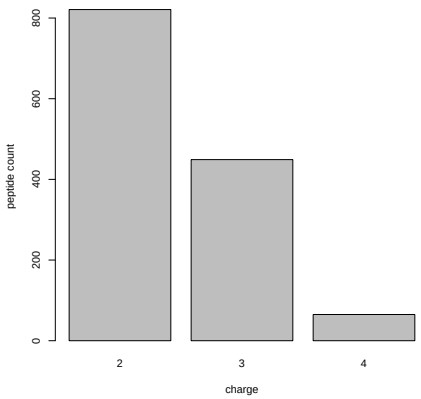


Figure 1: Charge distribution of peptide quantifications.

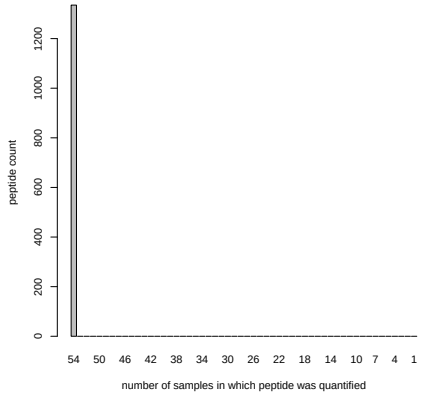


Figure 2: Frequency plot of peptide quantifications.

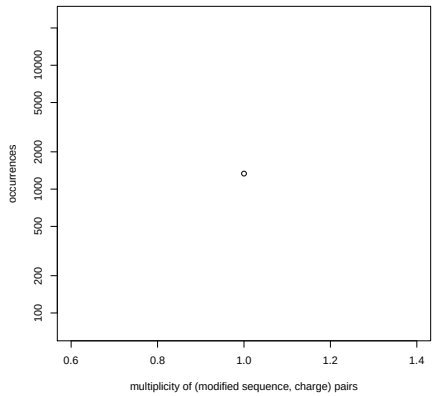


Figure 3: (modified sequence, charge) pair multiplicity vs frequency plot. Each peptide feature (characterised by a (possibly) modified peptide sequence and a charge state) should ideally occur only once in the analysis. In other words, peptides of multiplicity 1 should have a very high frequency. The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

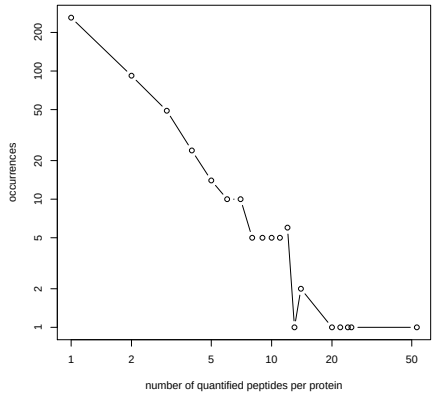


Figure 4: Number of quantified peptides per protein.

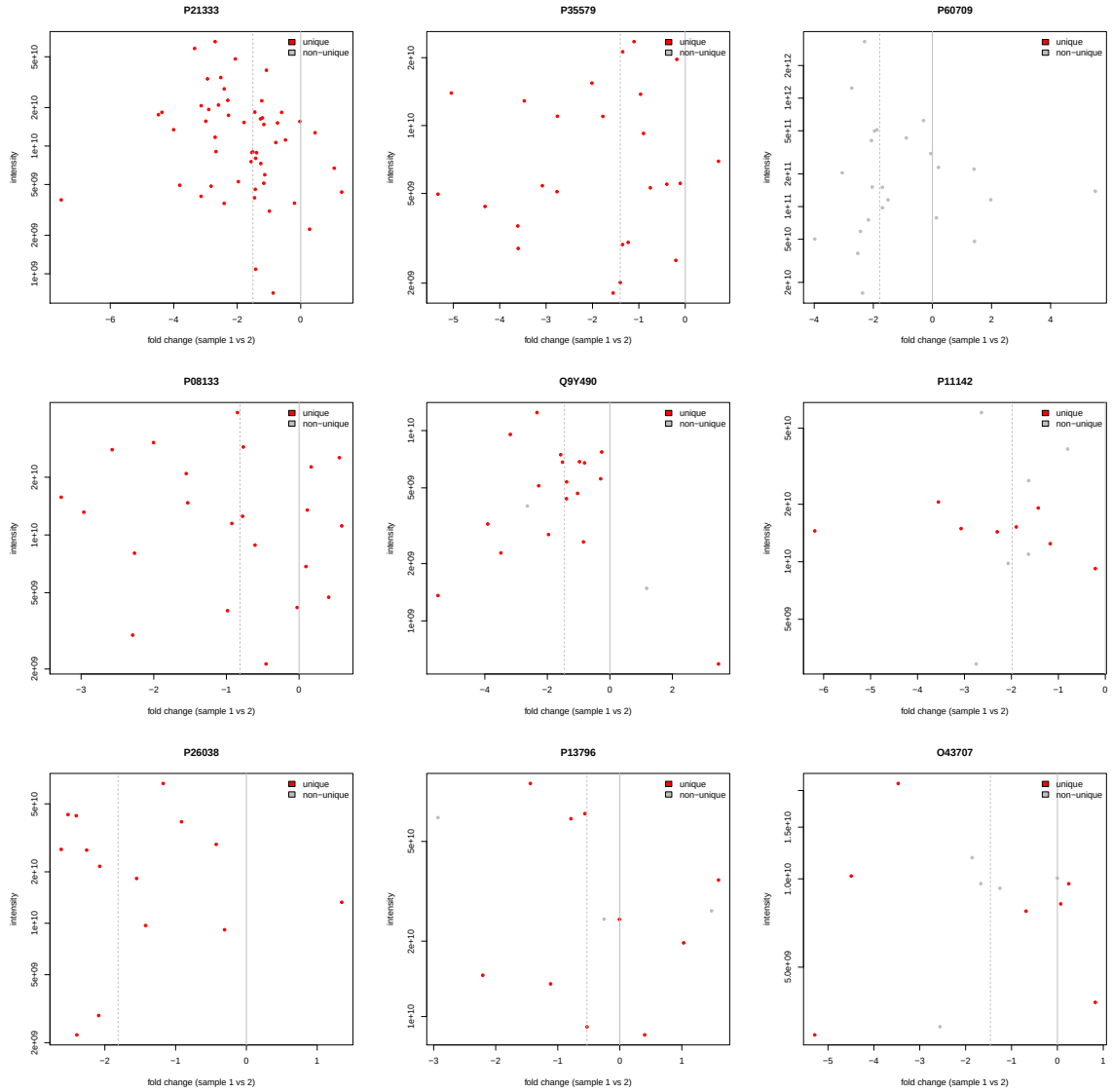
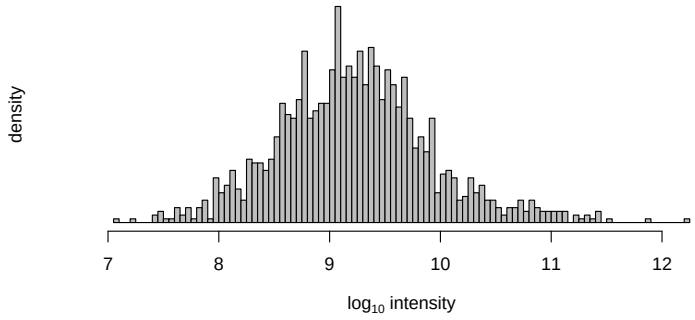
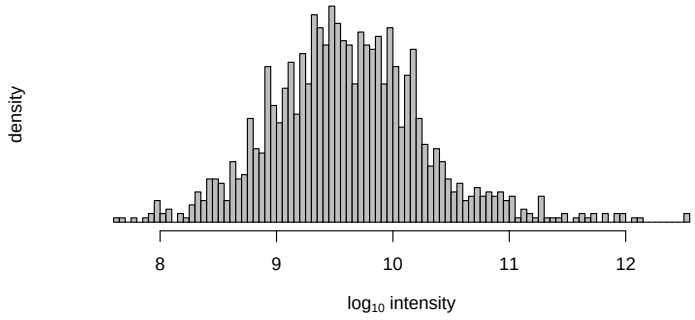


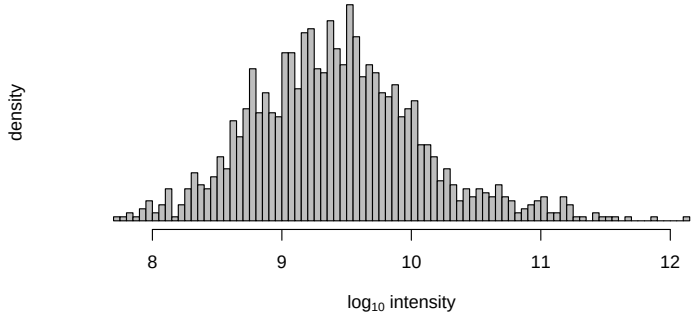
Figure 5: Fold changes of peptide abundances 1 and 2. For proteins with the largest number of quantified peptides.



(a) peptide abundances 1, median(intensity) $= 1,605,469,952$



(b) peptide abundances 2, median(intensity) $= 3,819,539,968$



(c) peptide abundances 3, median(intensity) $= 2,497,959,936$

Figure 6: peptide abundance distributions.

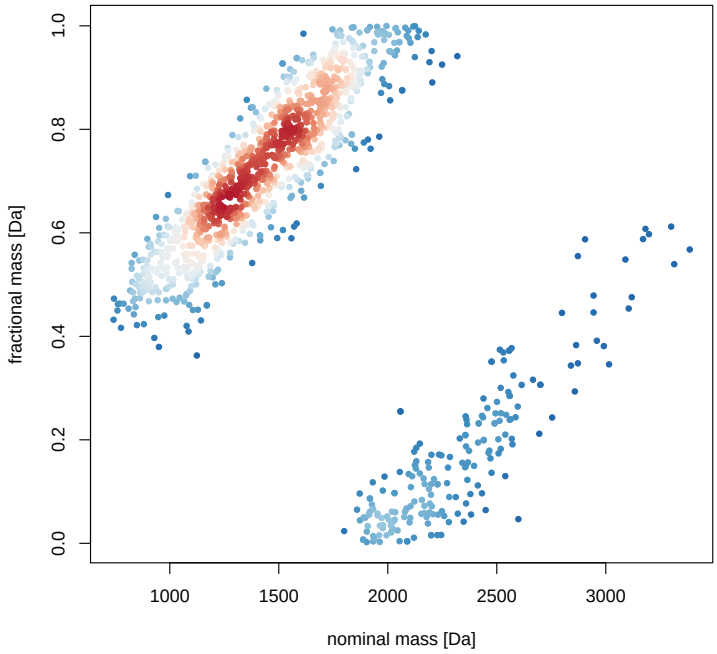


Figure 7: Kendrick nominal fractional mass plot

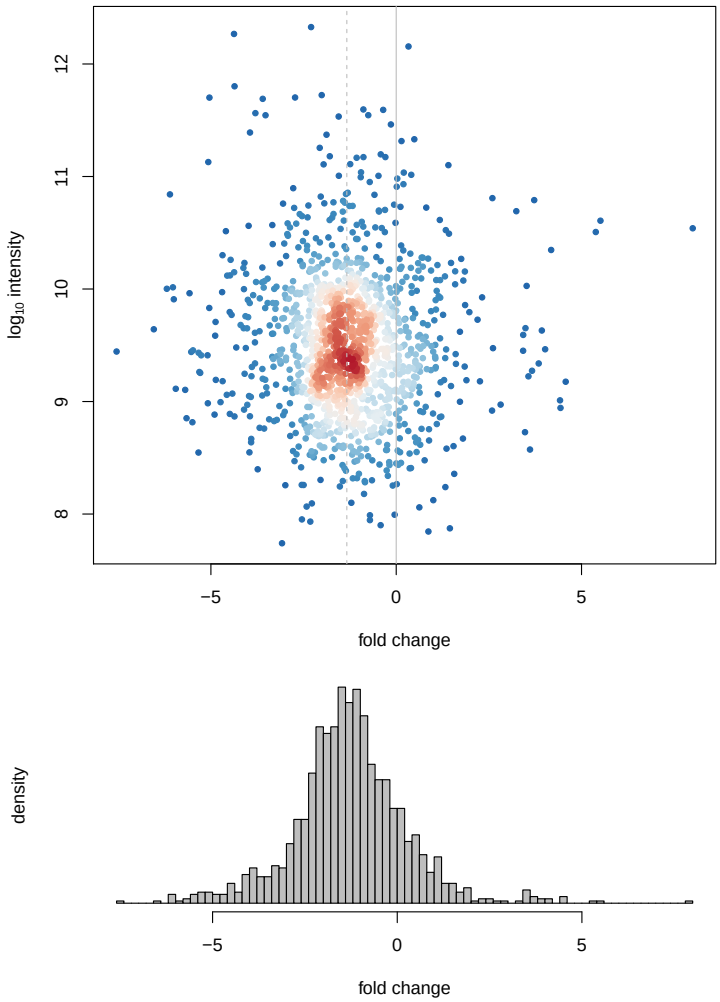


Figure 8: Fold changes of peptide abundances 1 and 2.
median(fc) = −1.3328 sd(fc) = 1.5445

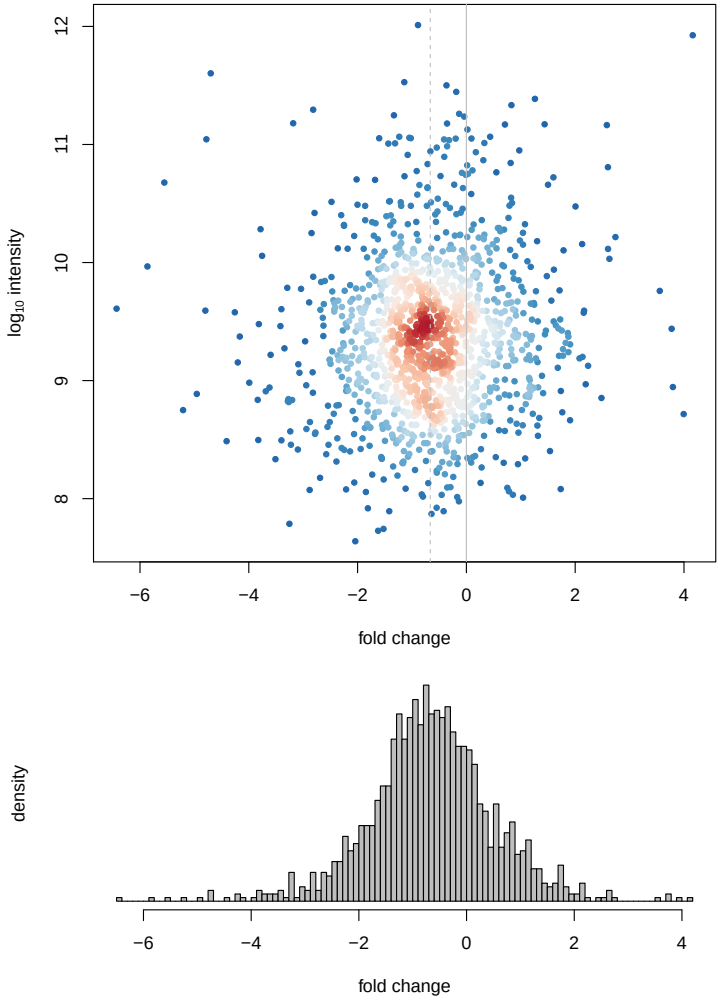


Figure 9: Fold changes of peptide abundances 1 and 3.
median(fc) = −0.6641 sd(fc) = 1.1804

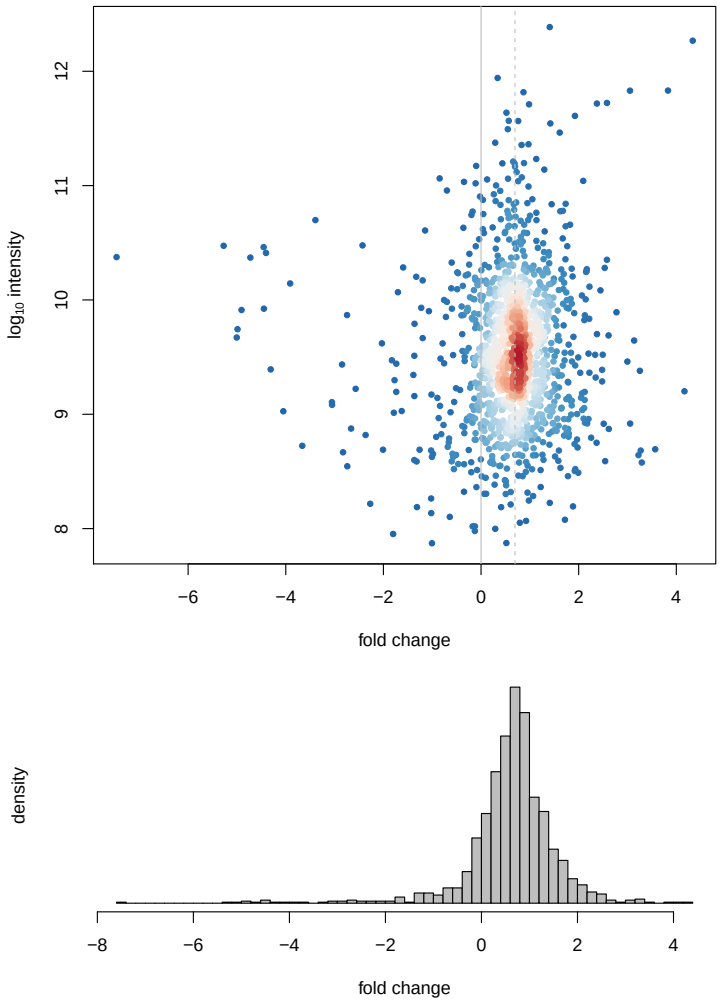


Figure 10: Fold changes of peptide abundances 2 and 3.
median(fc) = 0.6958 sd(fc) = 0.9636

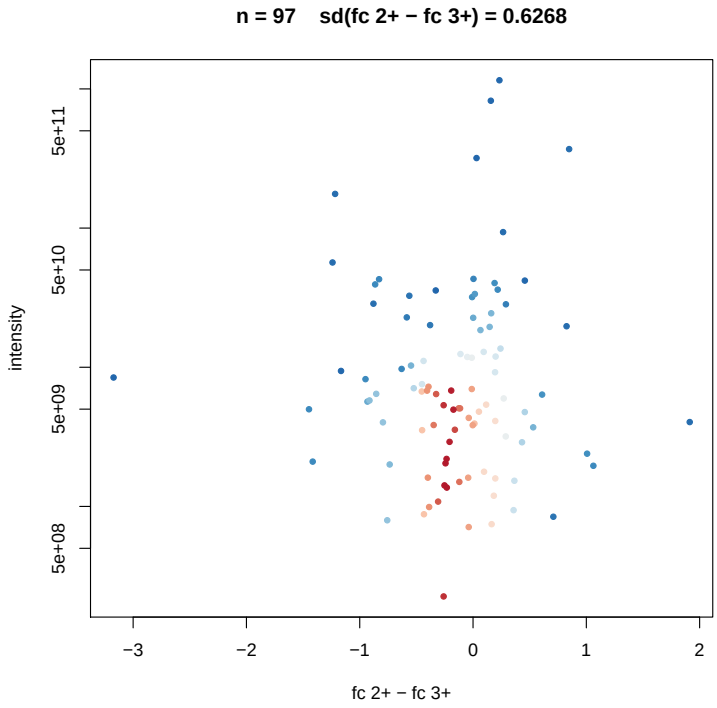


Figure 11: Fold changes of the same peptide in charge 2+ and 3+ are expected to be identical. Here we plot the difference of the 2+ and 3+ fold changes of sample 1 vs. sample 2 of all peptides which were identified and quantified in both charge states.

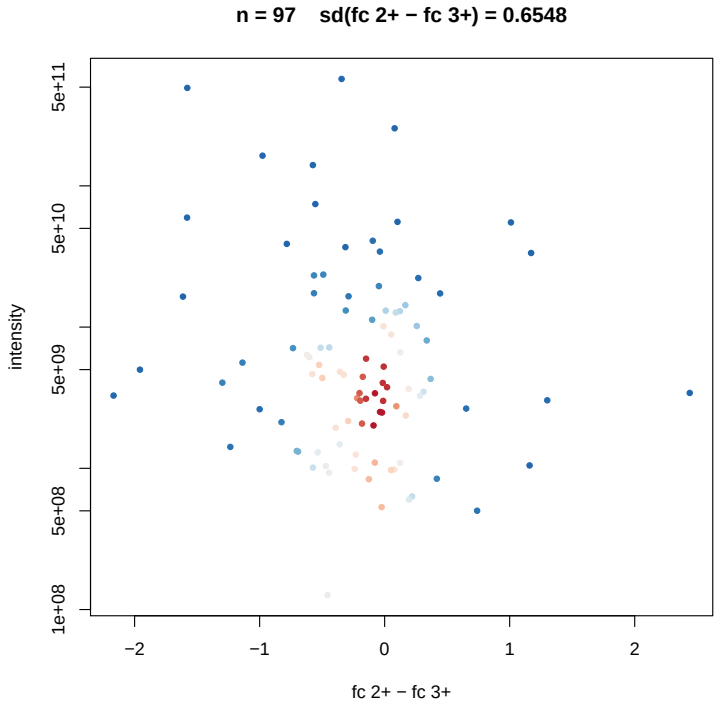


Figure 12: Fold changes of the same peptide in charge 2+ and 3+ are expected to be identical. Here we plot the difference of the 2+ and 3+ fold changes of sample 1 vs. sample 3 of all peptides which were identified and quantified in both charge states.

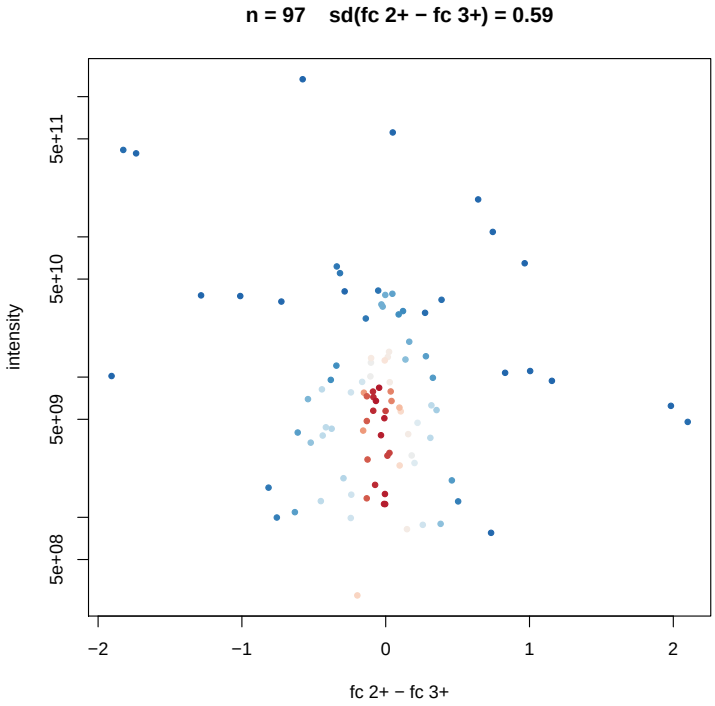


Figure 13: Fold changes of the same peptide in charge 2+ and 3+ are expected to be identical. Here we plot the difference of the 2+ and 3+ fold changes of sample 2 vs. sample 3 of all peptides which were identified and quantified in both charge states.

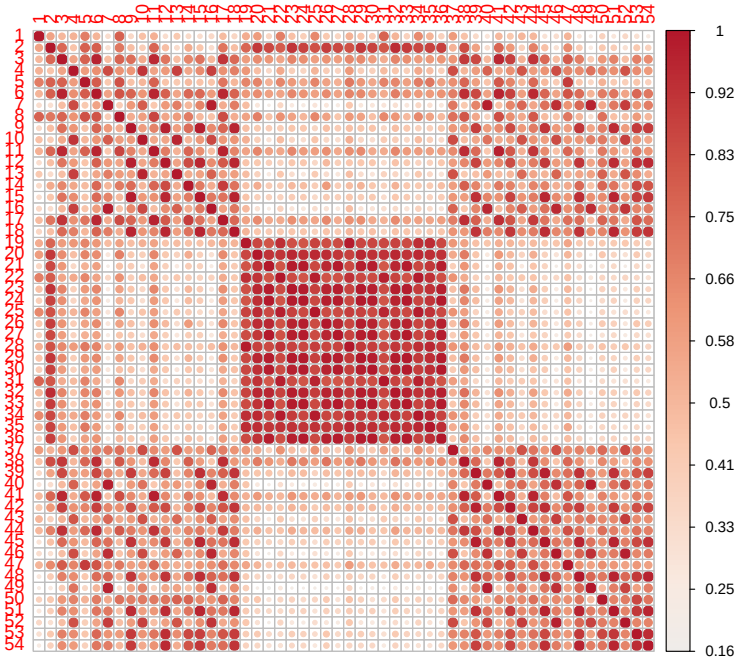


Figure 14: Pearson correlation of all peptide abundances. (min correlation = 0.1622, median correlation = 0.5936, max correlation = 1)

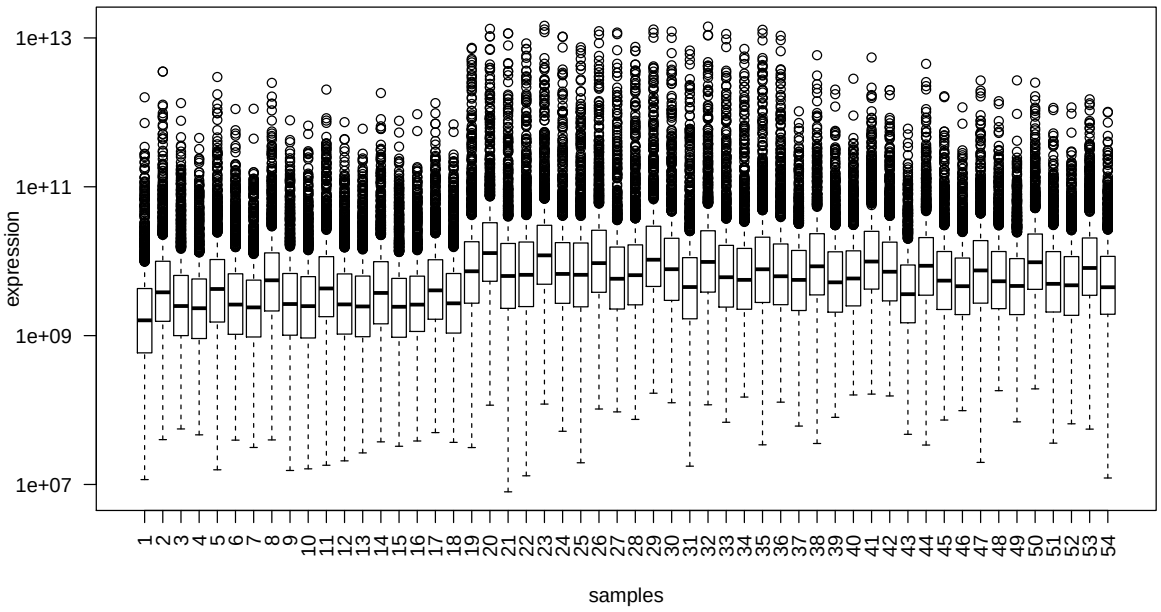


Figure 15: Boxplot of all peptide abundances.

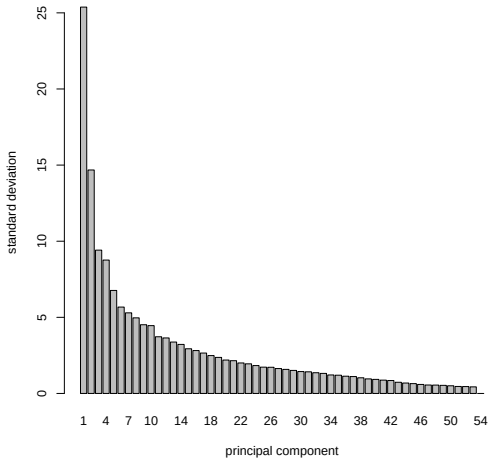


Figure 16: Standard deviation of all principal components.

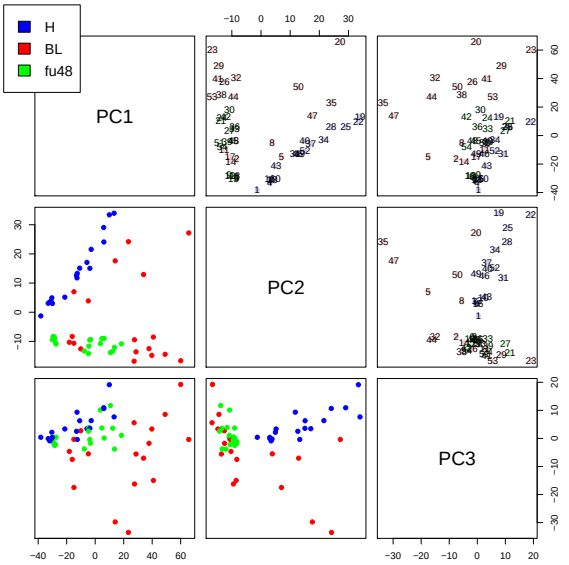


Figure 17: Principal Component Analysis of all peptides with complete quantifications. Any peptides with one or more missing values are ignored. The numbers in the upper right panels correspond to the sample IDs.

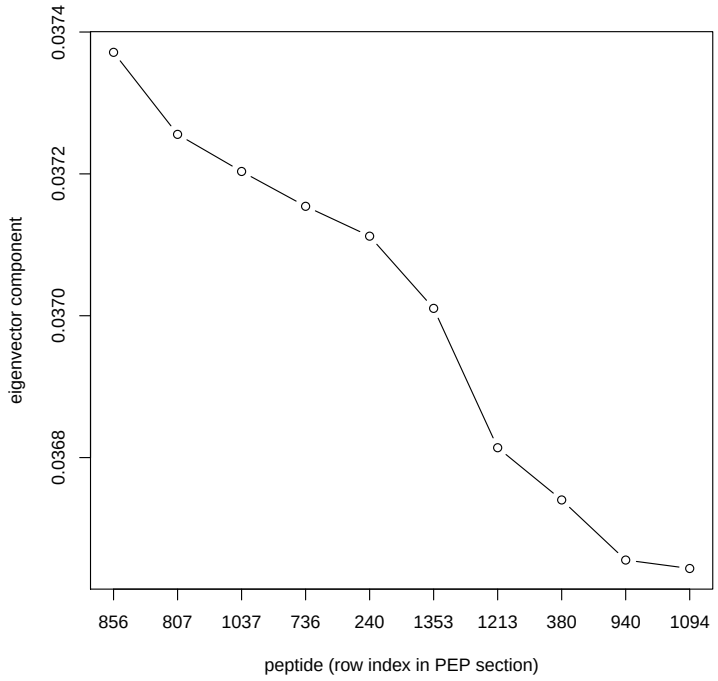


Figure 18: Most important contributions to the first principal component.

row index	modified sequence	accession	charge	retention time	m/z
856	LVPFDHAESTYGLYR	O95336	3.00	6753.43	589.96
807	TTPPVLDSDGSFFLYSK	P01857	2.00	9523.72	937.46
1037	VLKQVHPDTGISSK	P62807	2.00	1911.32	754.92
736	LYSILGTTLKDEGK	O75083	2.00	6063.81	769.43
240	FLPSELRDEH	Q9Y490	2.00	3804.75	621.81
1353	YGFIEGHVVIPR	P16070	3.00	6095.82	462.92
1213	TPAQYDASELK	P07355	2.00	3190.51	611.80
380	TSASIILR	P17987	2.00	3663.84	430.76
940	ILYSQC(Methylthio)GDVM(Ox...	P14649	2.00	5333.98	673.80
1094	ERQEAEEAKEALLQASR	P26038	3.00	4365.68	653.34

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

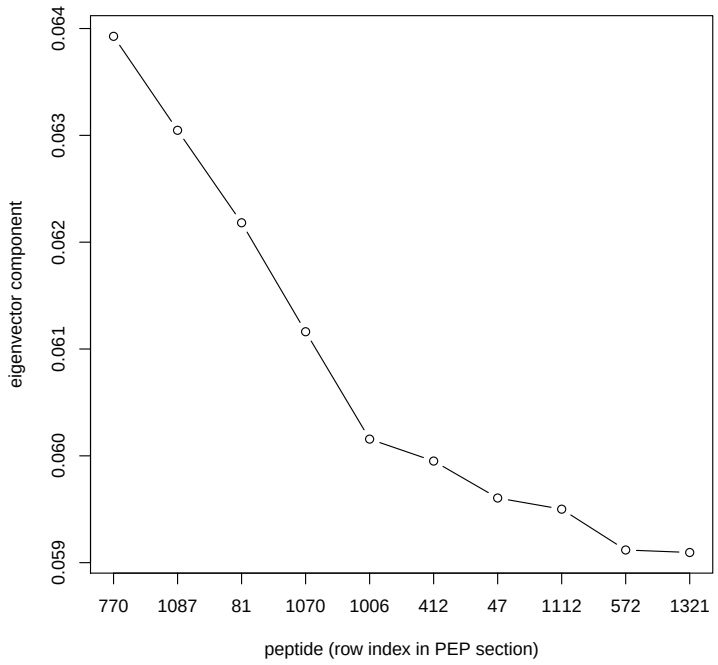


Figure 19: Most important contributions to the second principal component.

row index	modified sequence	accession	charge	retention time	m/z
770	GAVDGGLSIPHSTK	P46777	2.00	3445.54	669.85
1087	AIVAIENPADVSVISSR	P08865	2.00	8158.61	870.98
81	NVHGINFVSPVR	P53634	3.00	4626.45	446.91
1070	SKDIVLVAYSALGSQR	P42330	3.00	7358.33	569.65
1006	IAQSDYIPTQQDVLR	P04899	2.00	6684.21	873.95
412	LM(Oxidation)VALAK	P07355	2.00	3119.97	381.23
47	LLDAVDTYIPVPAR	P49411	2.00	9218.90	771.93
1112	TPALVNAAVTYSKPR	O75964	3.00	4964.94	529.97
572	IKIGDPLLEDTR	P49189	3.00	5956.77	457.26
1321	SGDSEVYQLGDVSQK	Q04837	2.00	5178.78	806.38

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

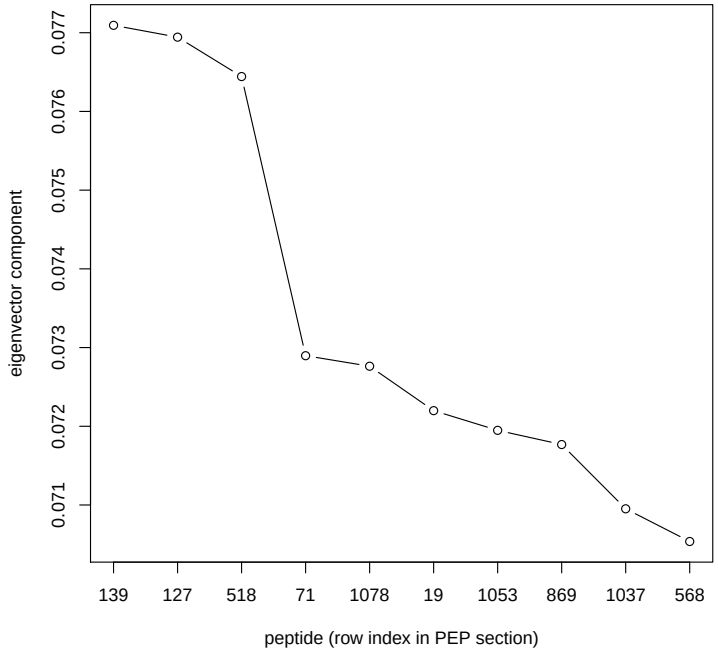


Figure 20: Most important contributions to the third principal component.

row index	modified sequence	accession	charge	retention time	m/z
139	VTAPDVDLHLKAPK	Q09666	3.00	4409.15	501.96
127	KDDLGDTNLHDYLR	Q9NUV9	3.00	5318.69	558.94
518	GFGFVLFK	Q14103	2.00	9123.27	457.76
71	IFVGGLSPDTPEEK	Q14103	2.00	6171.10	744.88
1078	TFVNITPAEVGVLVGKDR	P07737	3.00	8764.50	639.03
19	TIISYIDEQFER	Q15019	2.00	9451.35	757.38
1053	DREVGIPPEQSLETAK	P61158	2.00	4599.94	884.96
869	LAQAAQSSVATITR	Q9Y490	2.00	3767.92	708.89
1037	VLKQVHPDTGISSK	P62807	2.00	1911.32	754.92
568	HIYYITGETKDQVANSAFVER	P07900	4.00	5448.50	611.06

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

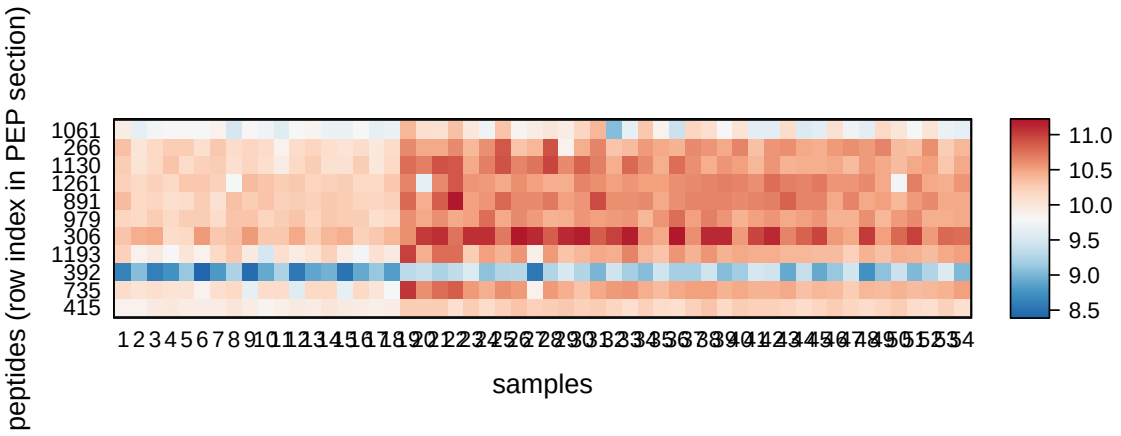


Figure 21: Logarithmic peptide abundances for all peptides of interest.

row index	modified sequence	accession	charge	retention time	m/z
1061	SSAAPPPPPR(Label:13C(6)15...	STD_01	2.00	1659.92	493.77
266	HVLTSIGEK(Label:13C(6)15N...	STD_03	2.00	2127.71	496.29
1130	IGDYAGIK(Label:13C(6)15N(...	STD_05	2.00	3096.71	422.74
1261	TASEFDSAIAQDK(Label:13C(6...	STD_06	2.00	4266.53	695.83
891	SAAGAFGPELSR(Label:13C(6)...	STD_07	2.00	4457.27	586.80
979	ELGQSGVDTYLQTK(Label:13C(...	STD_08	2.00	5741.14	773.90
306	GLILVGGYGTR(Label:13C(6)1...	STD_09	2.00	6431.53	558.33
1193	GILFVGSGVSGGEEGAR(Label:1...	P52209	2.00	6781.34	801.41
392	GILFVGSGVSGGEEGAR	P52209	2.00	6780.92	796.41
735	SFANQPLEVVYSK(Label:13C(6...	STD_11	2.00	6787.30	745.39
415	ELASGLSFPVGFK(Label:13C(6...	STD_14	2.00	9083.08	680.37

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	3.00	8103.29	630.69

Table 7: Proteins of interest.

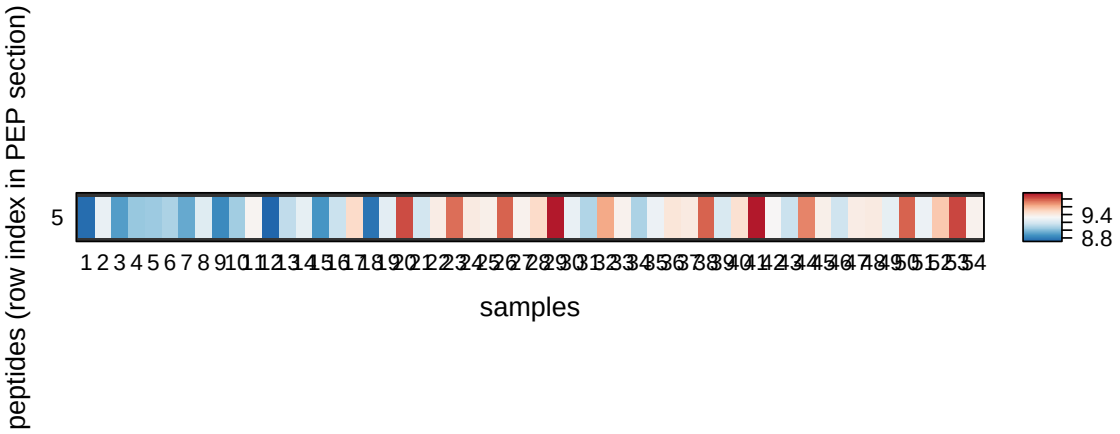


Figure 22: Logarithmic peptide abundances for all proteins of interest.

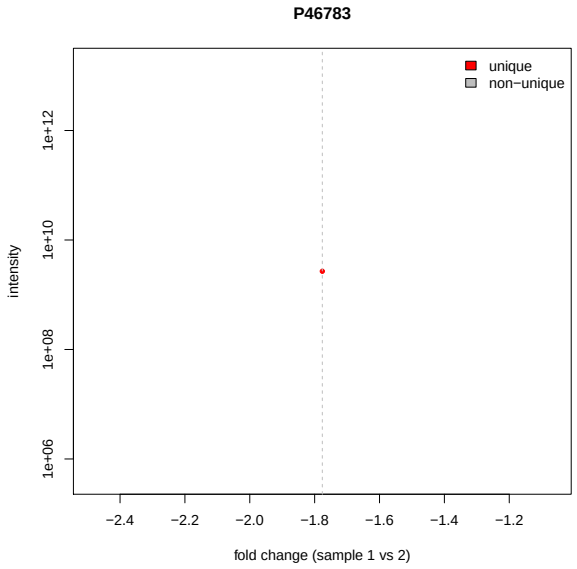


Figure 23: Fold changes of peptide abundances 1 and 2 for first protein of interest.