

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
identified (total)	1,335
identified (unique modified)	1,221
identified (unique stripped)	1,212

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.

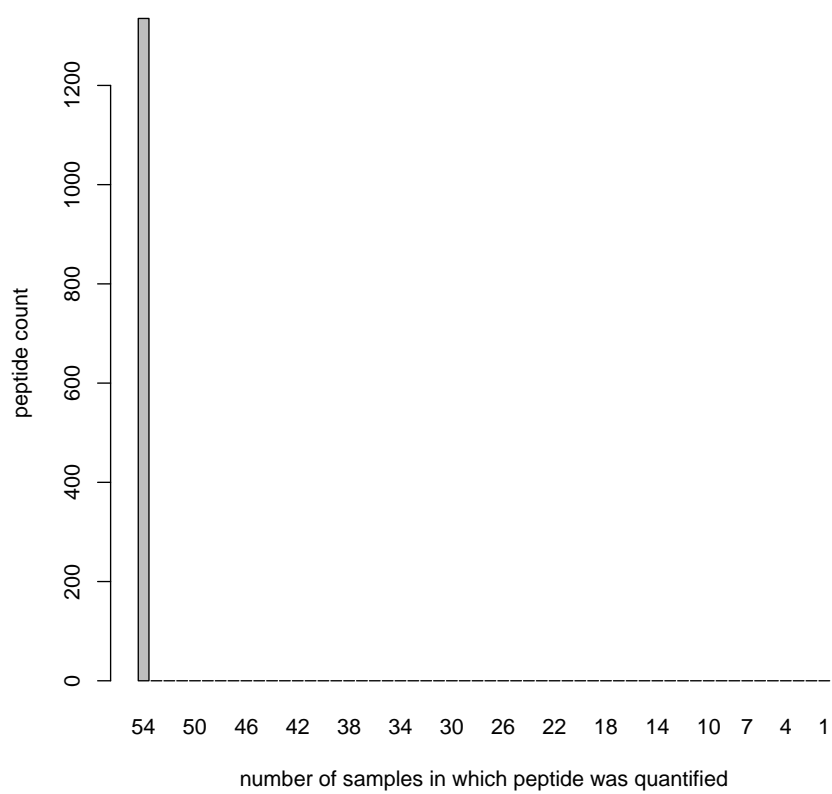
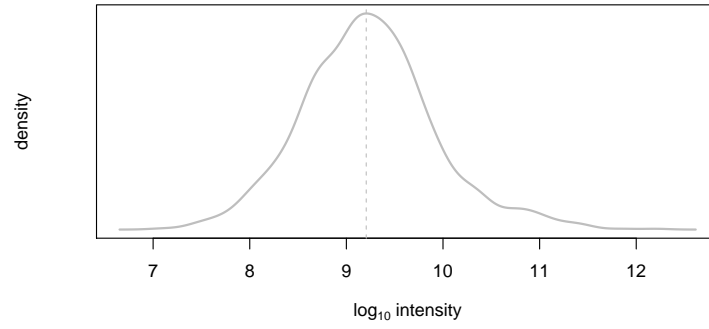


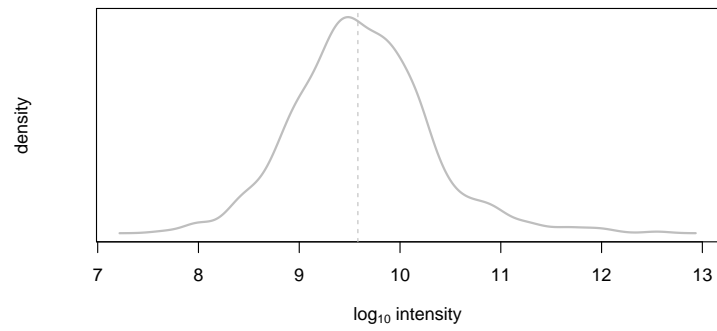
Figure 1: Frequency plot of peptide quantifications.



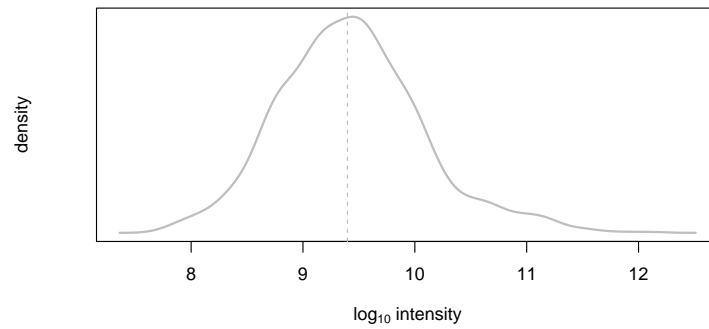
Figure 2: (modified sequence, charge) pair multiplicity vs frequency plot. Each peptide feature (characterised by a (possibly) modified peptide sequence and a charge state) should ideally occur only once in the analysis. In other words, peptides of multiplicity 1 should have a very high frequency. The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



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



(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 3: peptide abundance distributions.

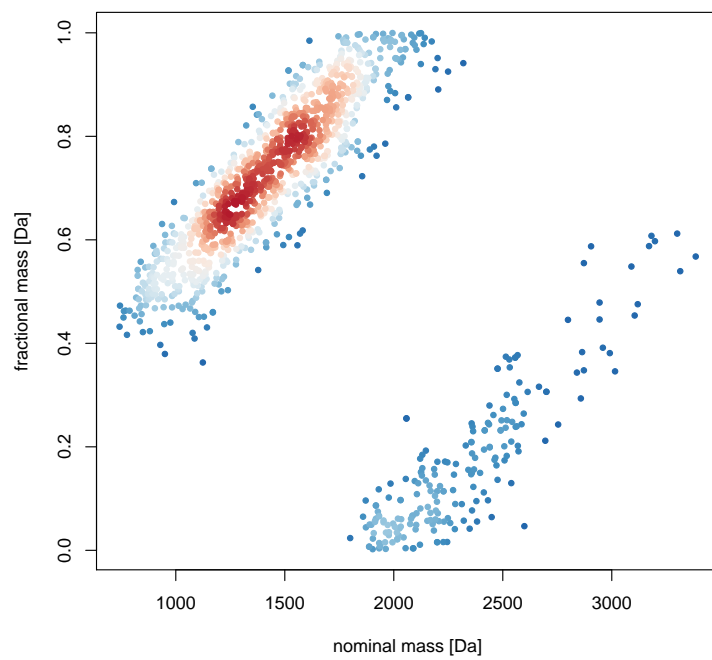


Figure 4: Kendrick nominal fractional mass plot

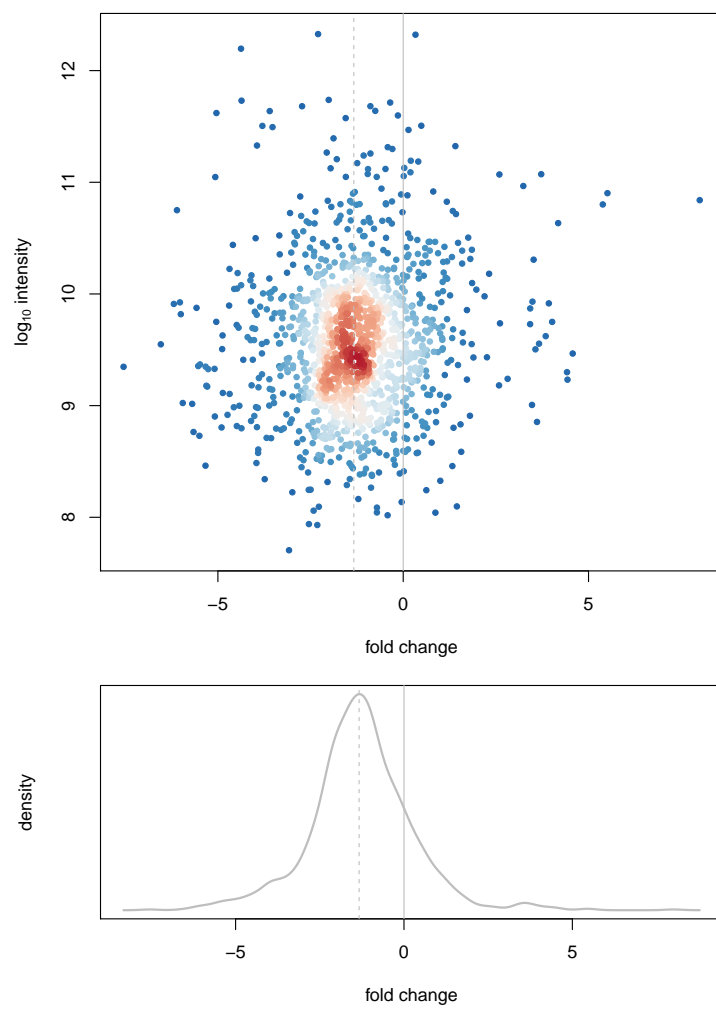


Figure 5: Fold changes of peptide abundances 1 and 2.
 $\text{median}(\text{fc}) = -1.3328$ $\text{sd}(\text{fc}) = 1.5445$

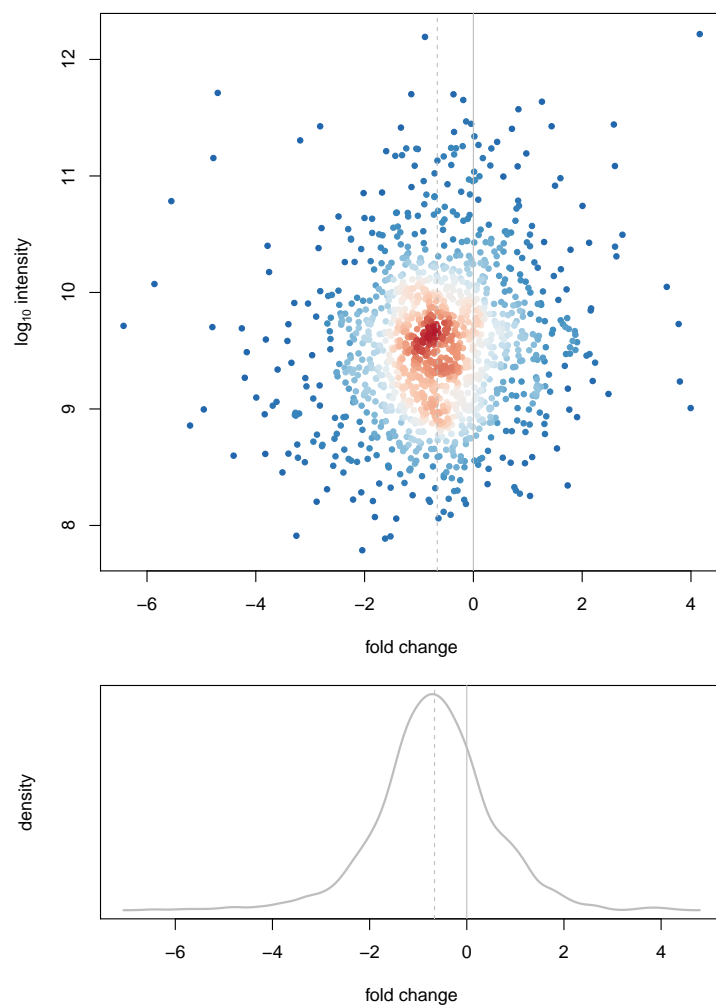


Figure 6: Fold changes of peptide abundances 1 and 3.
 $\text{median}(\text{fc}) = -0.6641$ $\text{sd}(\text{fc}) = 1.1804$

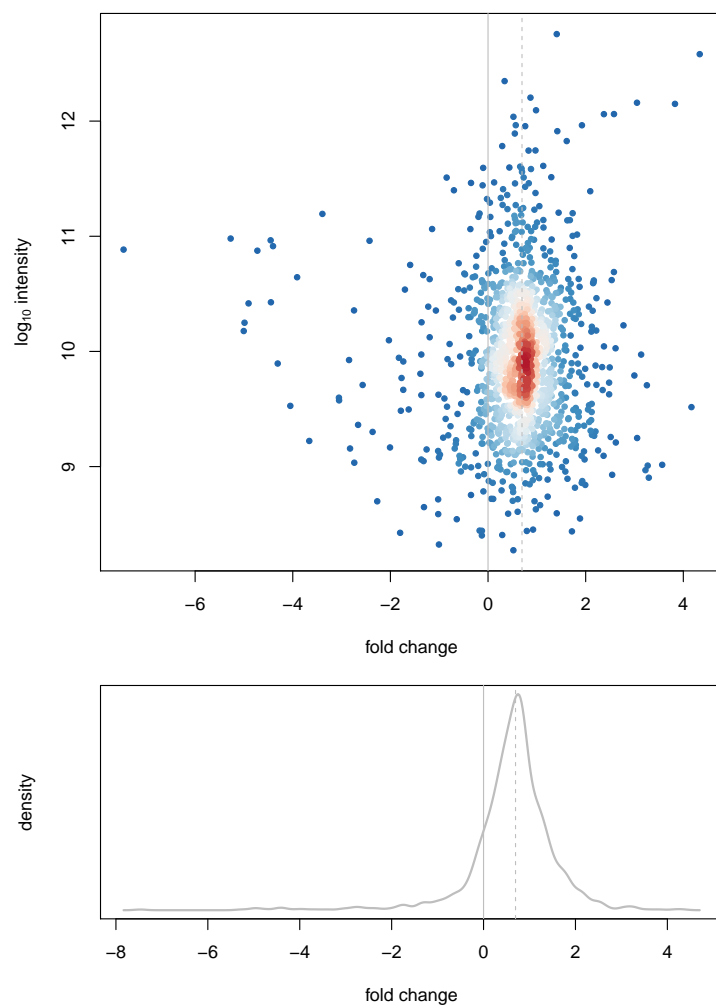


Figure 7: Fold changes of peptide abundances 2 and 3.
 $\text{median}(\text{fc}) = 0.6958$ $\text{sd}(\text{fc}) = 0.9636$

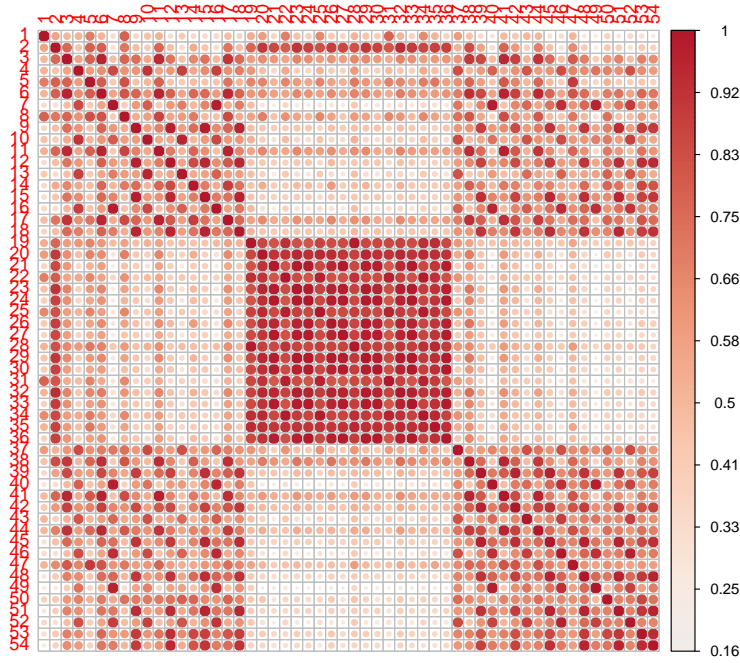


Figure 8: Pearson correlation of all peptide abundances. (min correlation = 0.1622, median correlation = 0.5936, max correlation = 1)

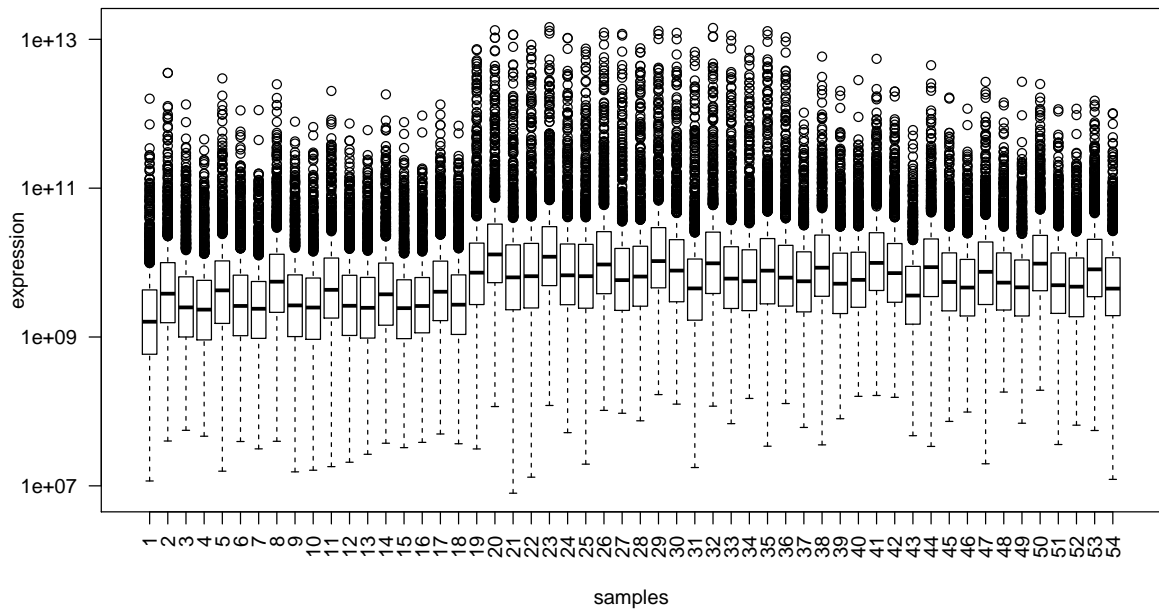
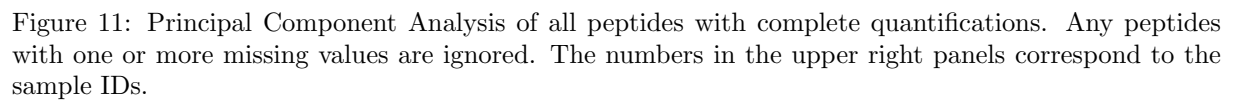


Figure 9: Boxplot of all peptide abundances.



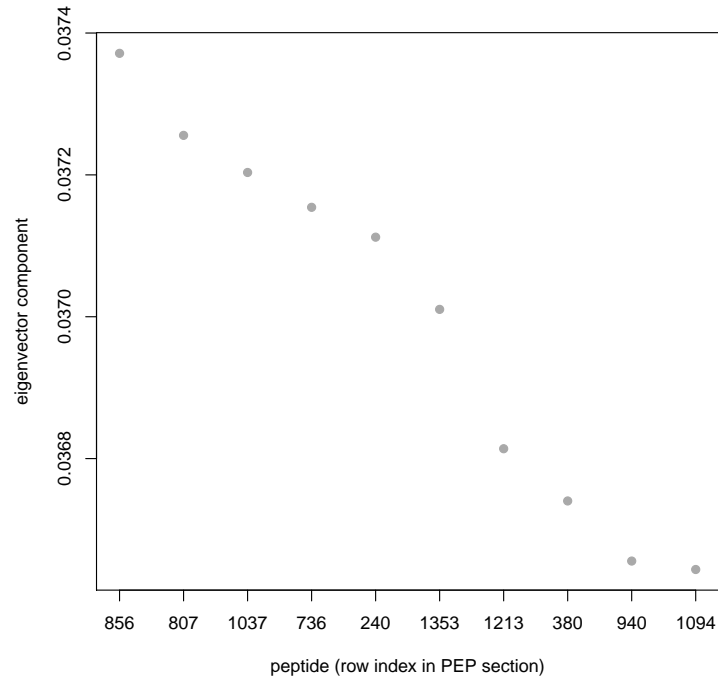


Figure 12: Most important contributions to the first principal component.

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 3: Most important contributions to the first principal component.

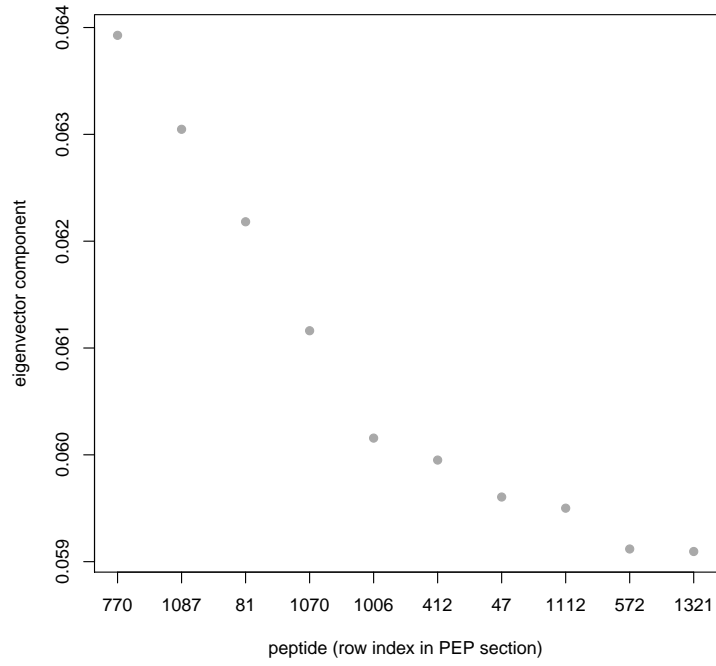


Figure 13: Most important contributions to the second principal component.

row index	modified sequence	accession	charge	retention time	m/z
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	LLDAVDTYIPVPAR	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 4: Most important contributions to the second principal component.

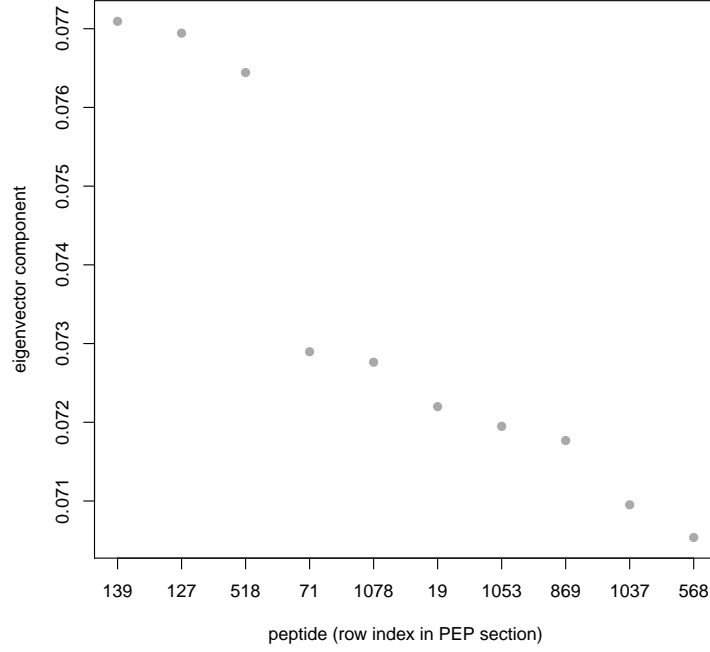


Figure 14: Most important contributions to the third principal component.

row index	modified sequence	accession	charge	retention time	m/z
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 5: Most important contributions to the third principal component.

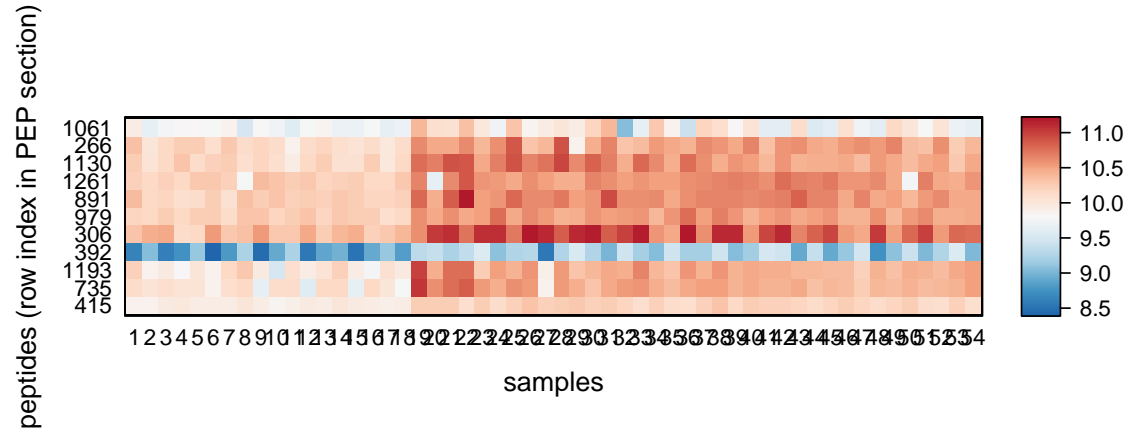


Figure 15: Logarithmic peptide abundances for all peptides of interest.

row index	modified sequence	accession	charge	retention time	m/z
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
392	GILFVGSGVSGGEEGAR	P52209	2	6780.92	796.41
1193	GILFVGSGVSGGEEGAR(Label:1...	P52209	2	6781.34	801.41
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 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

Table 7: Proteins of interest.

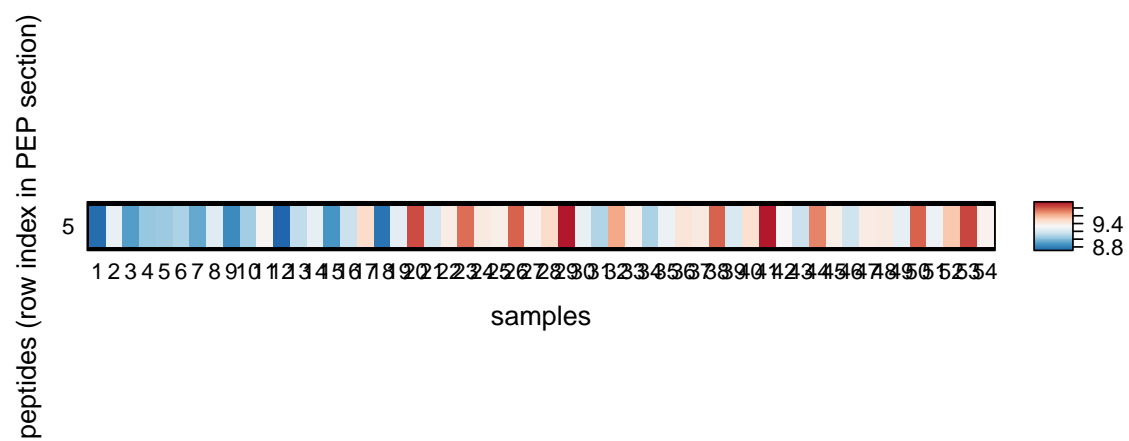


Figure 16: Logarithmic peptide abundances for all proteins of interest.