

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.

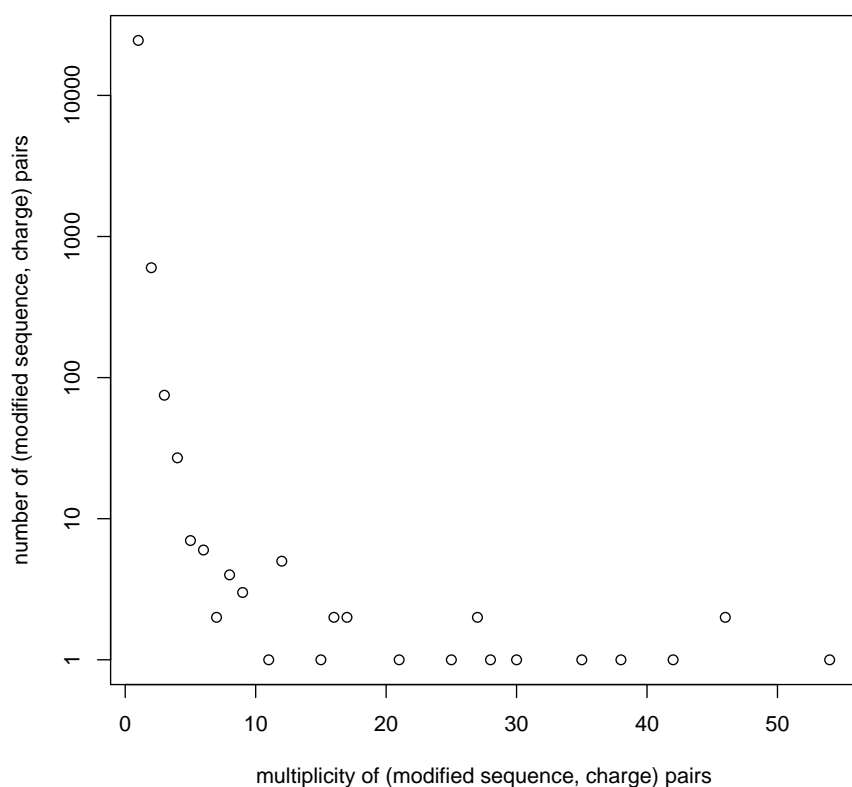
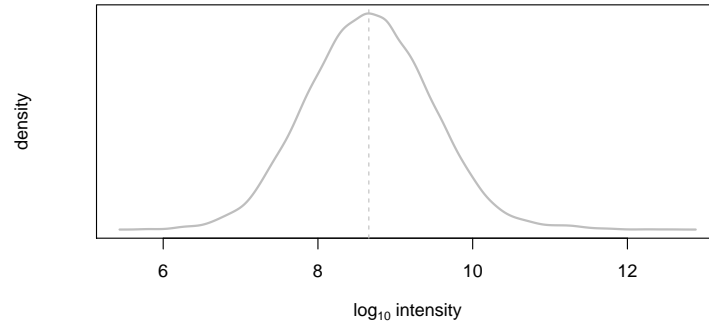
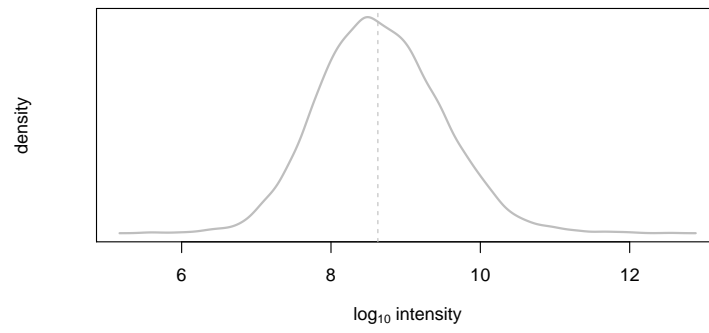


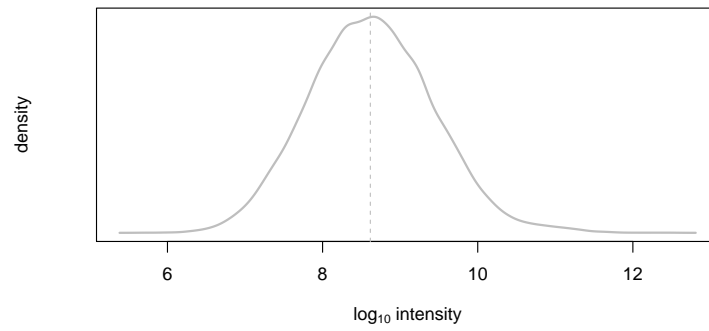
Figure 2: (modified sequence, charge) pair multiplicity vs frequency plot. Each peptide feature (characterised by a (possibly) modified peptide sequence and a charge state) should ideally occur only once in the analysis. In other words, peptides of multiplicity 1 should have a very high frequency. The 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, $\text{median}(\text{intensity}) = 424,578,000$



(c) peptide abundances 3, $\text{median}(\text{intensity}) = 412,578,512$

Figure 3: peptide abundance distributions.

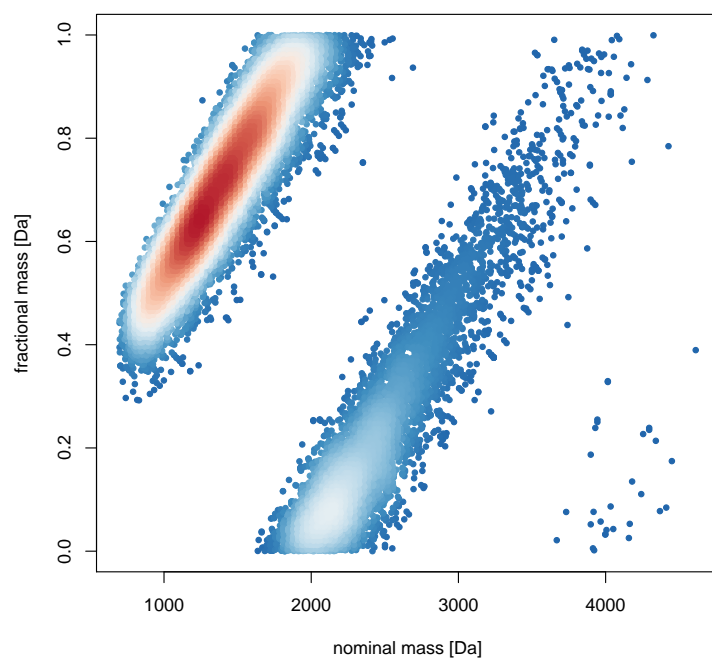


Figure 4: Kendrick nominal fractional mass plot

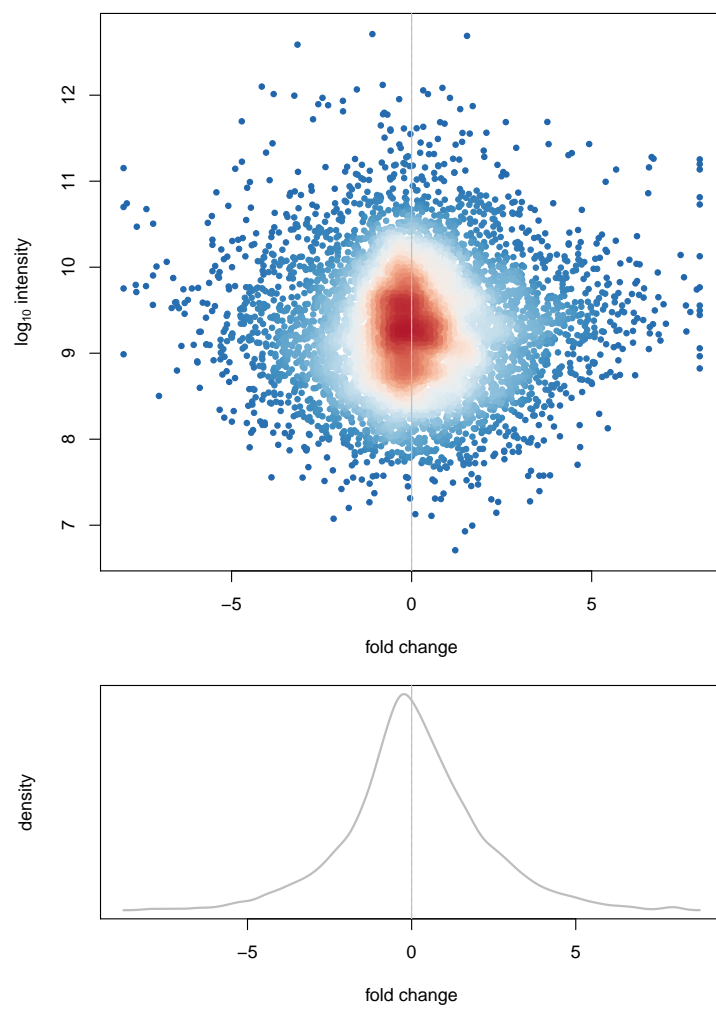


Figure 5: Fold changes of peptide abundances 1 and 2.
 $\text{median}(\text{fc}) = -0.0026$ $\text{sd}(\text{fc}) = 2.0776$

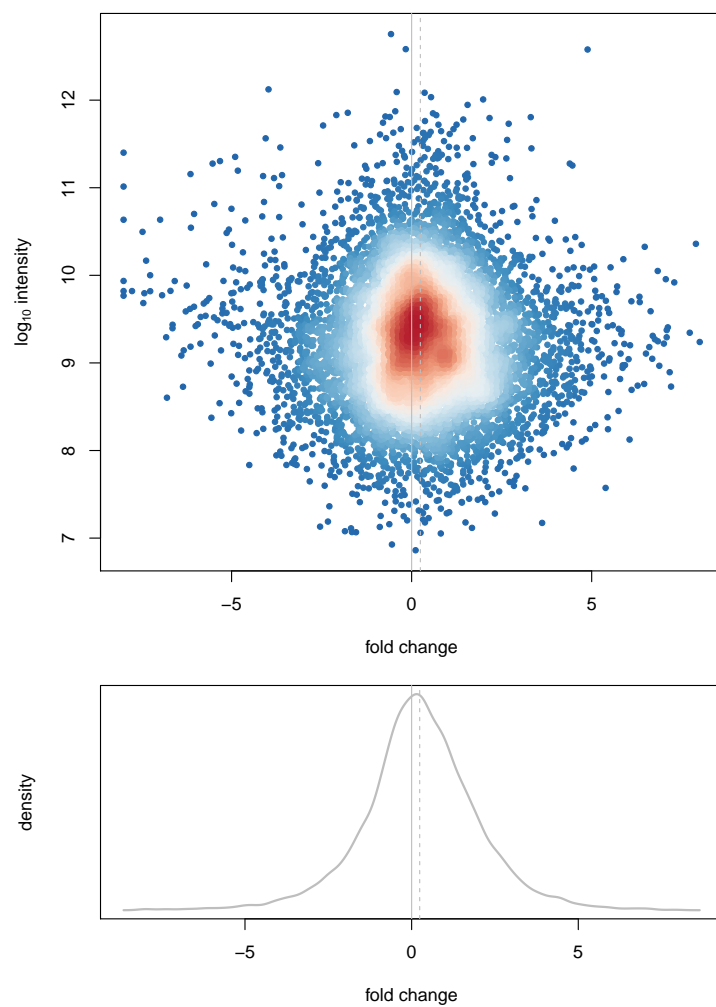


Figure 6: Fold changes of peptide abundances 1 and 3.
 $\text{median}(\text{fc}) = 0.2421$ $\text{sd}(\text{fc}) = 1.7661$

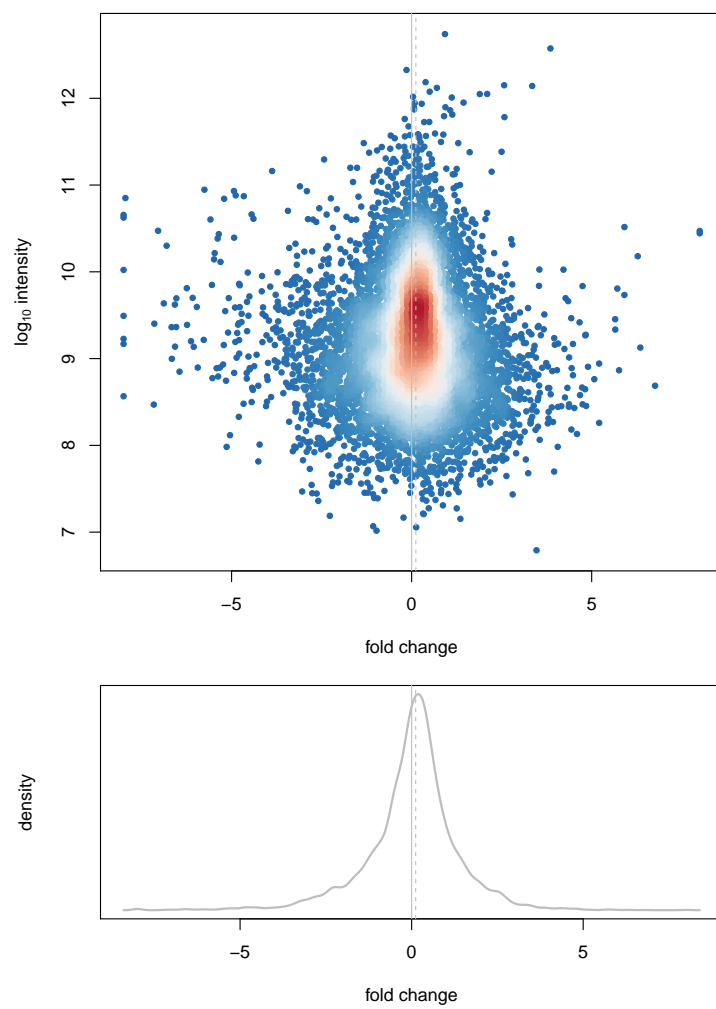


Figure 7: Fold changes of peptide abundances 2 and 3.
 $\text{median}(\text{fc}) = 0.1175$ $\text{sd}(\text{fc}) = 1.3543$

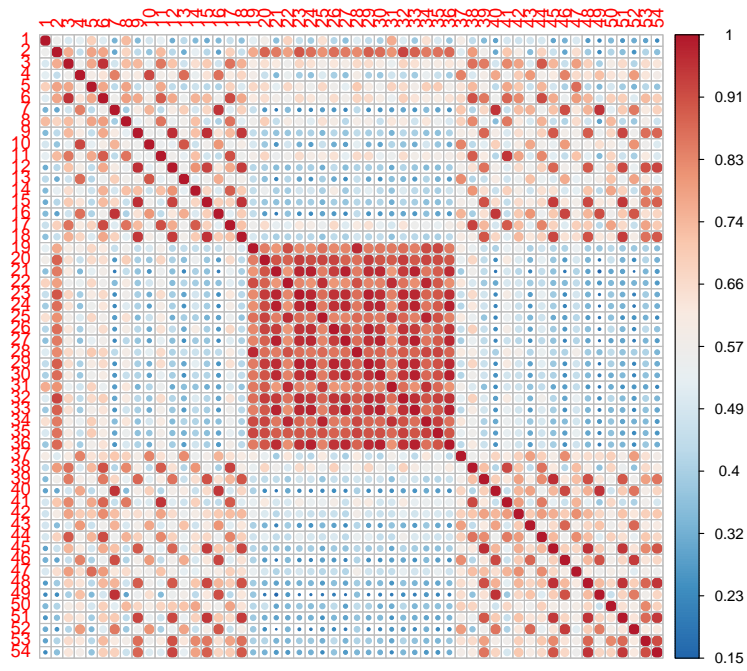


Figure 8: Pearson correlation of all peptide abundances. (min correlation = 0.1484, median correlation = 0.5701, max correlation = 1)

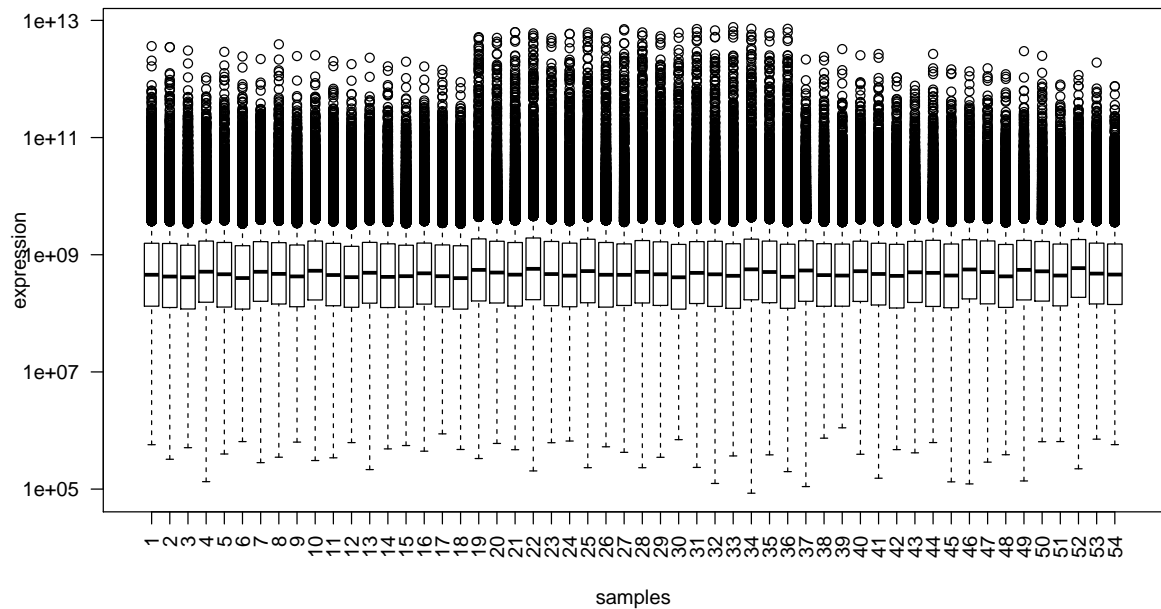


Figure 9: Boxplot of all peptide abundances.

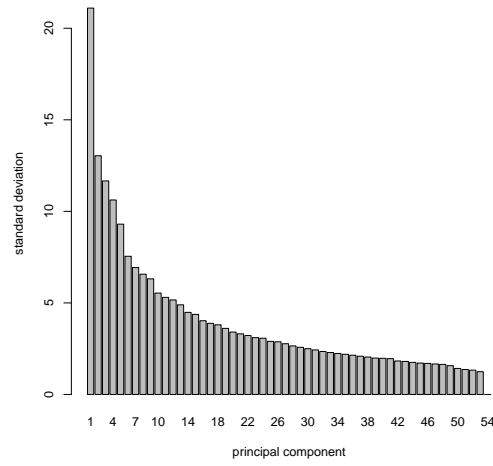


Figure 10: Standard deviation of all principal components.

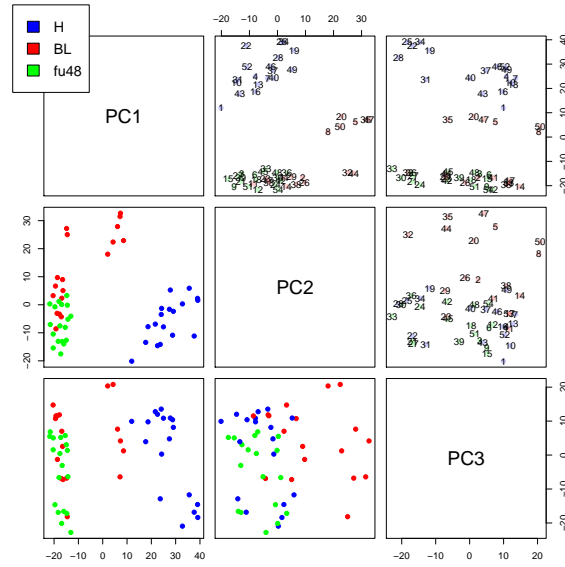


Figure 11: Principal Component Analysis of all peptides with complete quantifications. Any peptides with one or more missing values are ignored. The numbers in the upper right panels correspond to the sample IDs.

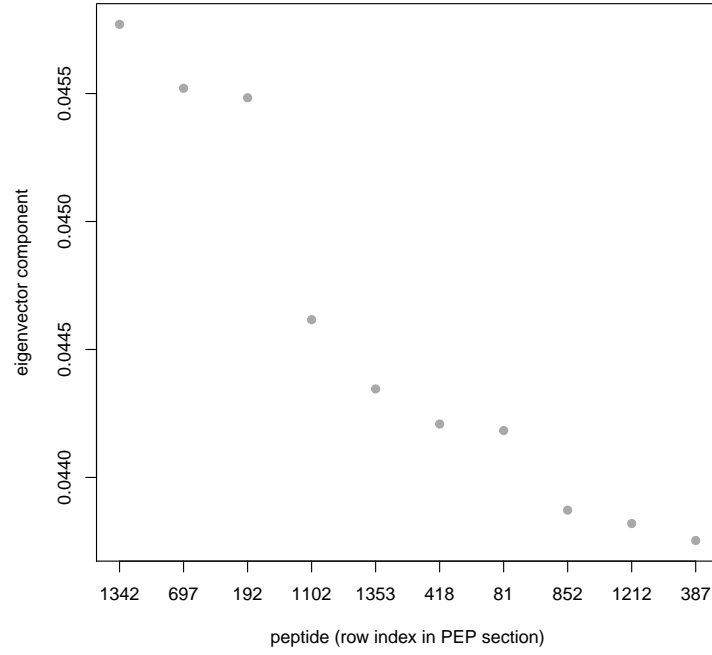


Figure 12: Most important contributions to the first principal component.

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.

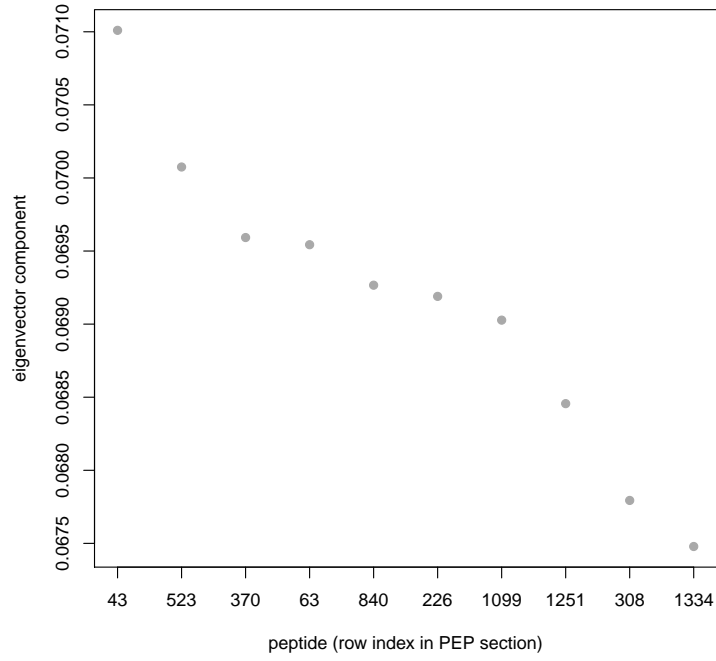


Figure 13: Most important contributions to the second principal component.

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.

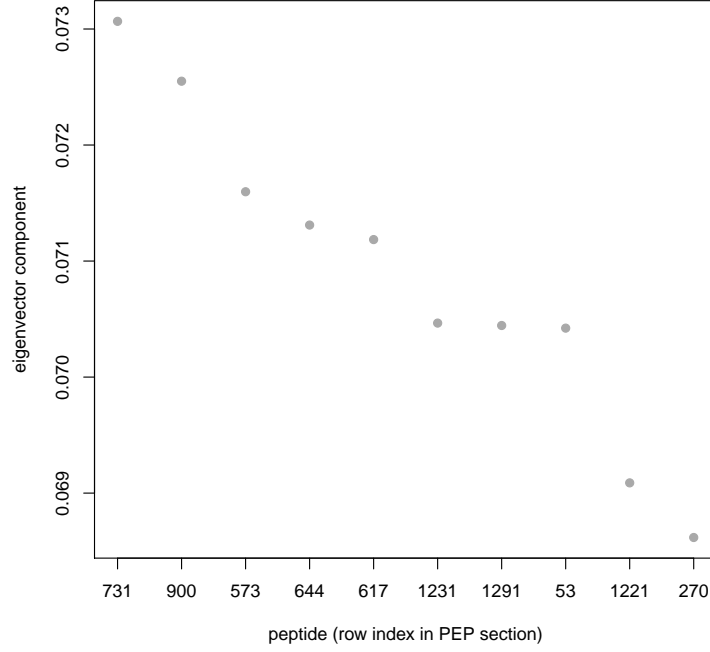


Figure 14: Most important contributions to the third principal component.

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.

modified sequence	accession	charge	retention time	m/z
LSLM(Oxidation)YAR	P78527	2	3727.04	435.23
LSLMYAR	P78527	2	4790.39	427.23
EQC(Methylthio)C(Methylth...	P62633	4	4025.06	454.93
EQC(Methylthio)C(Methylth...	P62633	3	4045.75	606.23
M(Oxidation)VQEAEKYKAEDEK...	P11142	4	1316.10	500.25
M(Oxidation)VQEAEKYKAEDEK...	P11142	3	1320.29	666.66
MVQEAEKYKAEDEKQR	P11142	3	1585.13	661.33
M(Oxidation)VQEAEKYKAEDEK...	P11142	2	1324.47	999.48
MVQEAEKYKAEDEKQR	P11142	4	1577.81	496.25
TVPF(C(Methylthio)STFAAFFT...	P29401	2	12736.46	820.88
GNFGGSFAGSFSGGAGGHAPGVAR	P52272	3	5570.46	678.99
GNFGGSFAGSFSGGAGGHAPGVAR	P52272	2	5569.35	1017.98
GNFGGSFAGSFSGGAGGHAPGVARK	P52272	4	4336.39	541.52
GNFGGSFAGSFSGGAGGHAPGVARK	P52272	3	4346.43	721.69

Table 6: Peptides of interest. Please note that the script requires a vector of *stripped* peptide sequences, but in the above table we list the *modified* peptide sequences.

modified sequence	accession	charge	retention time	m/z
AEAGAGSATEFQFR	P46783	2	5036.50	721.34
DYLHLPPEIVPATLR	P46783	3	9558.62	578.66
DYLHLPPEIVPATLR	P46783	2	9548.91	867.48
DYLHLPPEIVPATLRR	P46783	3	8103.29	630.69
DYLHLPPEIVPATLRR	P46783	4	8100.98	473.27
GYVKEQFAWR	P46783	3	4253.53	428.56
GYVKEQFAWR	P46783	2	4257.40	642.33
HFYWYLTNEGIIQYLR	P46783	3	9290.39	668.33
HPELADKNVPLHVM(Oxidation...	P46783	4	2806.75	465.25
IAIYELLFK	P46783	2	10732.68	555.33
IAIYELLFKEGVM(Oxidation)V...	P46783	3	10197.44	614.01
KAEAGAGSATEFQFR	P46783	2	3516.88	785.39
KAEAGAGSATEFQFR	P46783	3	3518.31	523.93
SAVPPGADKKAEAGAGSATEFQFR	P46783	4	4302.34	598.80
SAVPPGADKKAEAGAGSATEFQFR	P46783	3	4302.30	798.07
SRPETGRPRPK	P46783	2	1112.69	640.86
SRPETGRPRPK	P46783	3	1112.97	427.58
AADSQNSGEGNTGAAESSFSQEVSR	P12270	2	4519.04	1243.53
AALKQLQEIFYENYKK	P12270	4	6949.96	456.51
EGVQGPLNVSLSEEGKSQEQILEIL...	P12270	3	10181.28	951.51
EKEIAETRFEVAQVESLR	P12270	3	5813.97	712.04
EKGNEILELK	P12270	2	3452.76	586.83
FKVESEQQYFEIEKR	P12270	3	4954.28	654.00
FLADQQSEIDGLKGRHEK	P12270	4	3196.05	518.52
GIASDPTPTANIKPTPVVSTPSK	P12270	3	4902.51	789.09
GQNLLLTNLQTIQGILER	P12270	2	12445.40	1012.58
ILLSQTTGVAIPLHASSLDDVSLAS...	P12270	3	9456.43	945.52
ISTQLDFASK	P12270	2	4987.08	555.30
ITELQLKLESALTELEQLRK	P12270	4	10747.62	589.59
KLELDILPLQEANAELSEK	P12270	3	9473.26	718.40
KLENEVEQR	P12270	2	1635.88	572.80
LENEVEQR	P12270	2	1693.68	508.75
LESALTELEQLRK	P12270	3	6908.25	510.62
LLSEKEVHTK	P12270	2	1506.47	592.33

LQEQVTDLR	P12270	2	3580.96	551.30
LSQELEYLTEDVKR	P12270	3	6542.97	574.97
LSSQIEKLEHEISHLK	P12270	4	6322.55	473.51
LTIHAPPQELGPPVQR	P12270	3	5244.98	585.00
NLDVQLLDTK	P12270	2	6805.16	579.82
NLQEQTVQLQSELSR	P12270	2	6830.64	886.96
RPSTSQTVSTPAPVPVIESTEAEIA...	P12270	3	6727.12	899.14
SAADDSEAKSNELTR	P12270	3	1865.12	531.92
SAADDSEAKSNELTR	P12270	2	1834.45	797.37
SQEQILEILR	P12270	2	7860.87	614.85
TKEELEAEKR	P12270	2	1216.40	616.83
TLSSVQNEVQEALQR	P12270	2	7739.83	851.44
YLDEIVKEVEAK	P12270	3	7196.92	479.26

Table 7: Proteins of interest.