

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

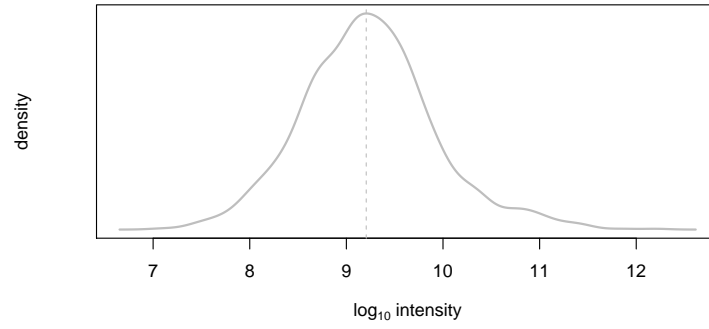
Table 2: Statistics of modifications.



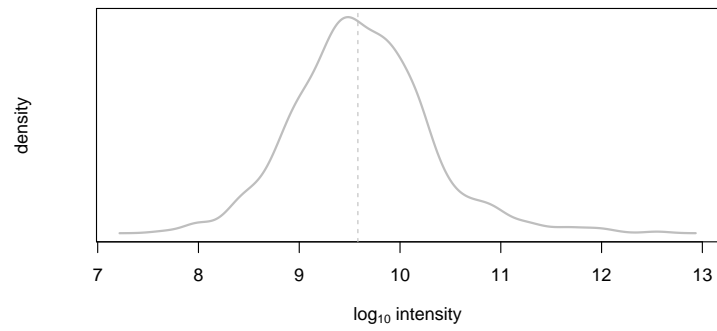
Figure 1: Frequency plot of peptide quantifications.



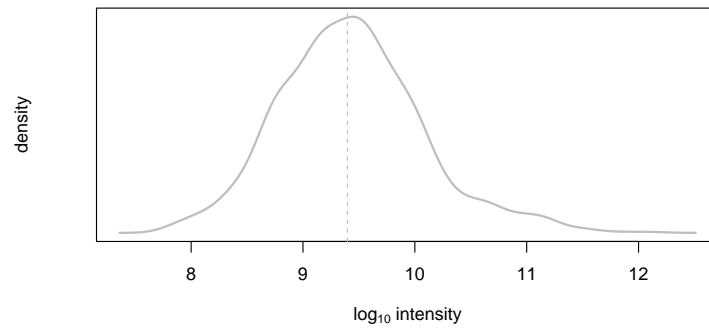
Figure 2: (modified sequence, charge) pair multiplicity vs frequency plot. Each peptide feature (characterised by a (possibly) modified peptide sequence and a charge state) should ideally occur only once in the analysis. In other words, peptides of multiplicity 1 should have a very high frequency. The 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.

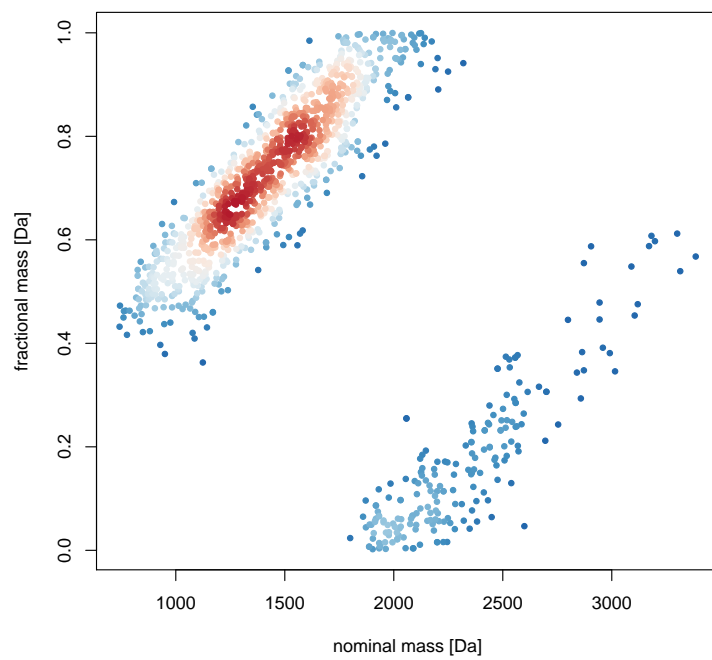


Figure 4: Kendrick nominal fractional mass plot

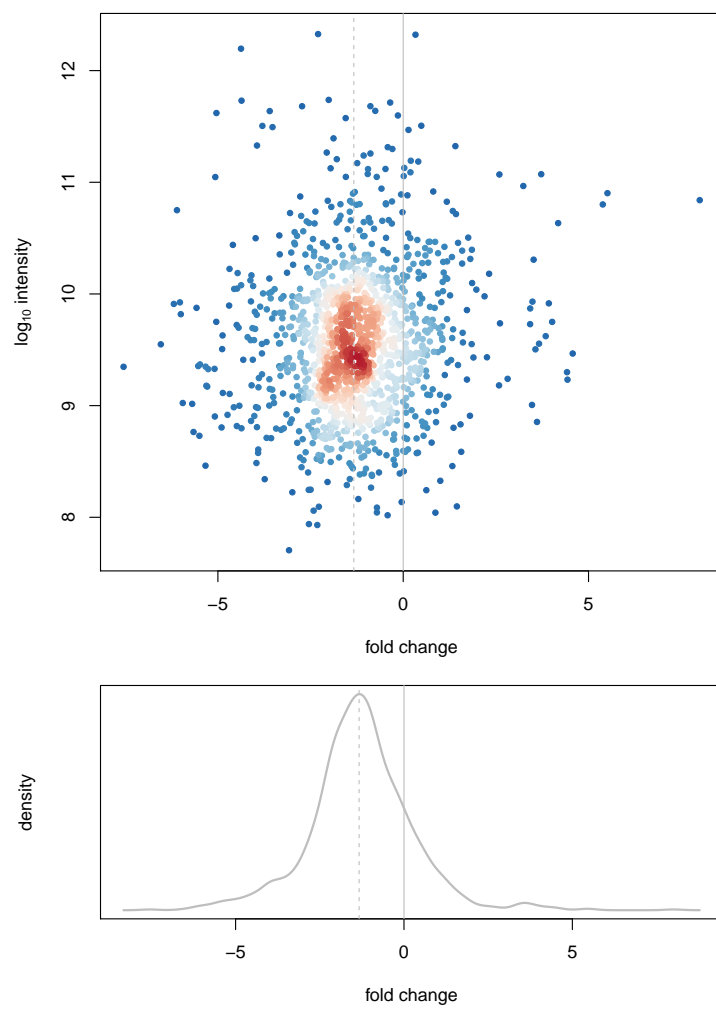


Figure 5: Fold changes of peptide abundances 1 and 2.
 $\text{median}(\text{fc}) = -1.3328$ $\text{sd}(\text{fc}) = 1.5445$

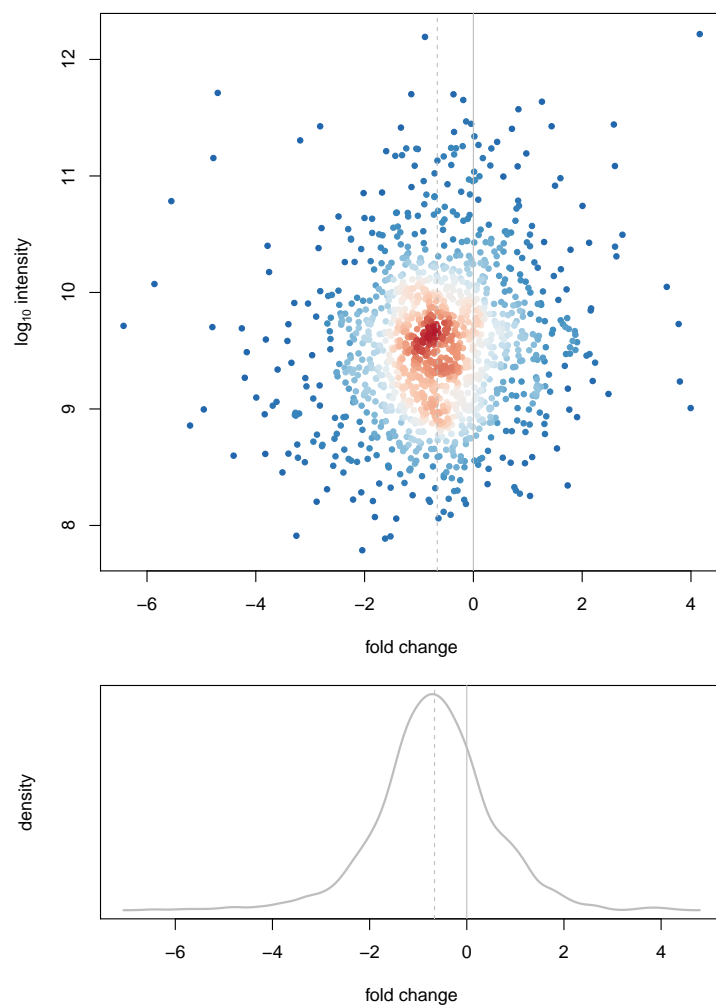


Figure 6: Fold changes of peptide abundances 1 and 3.
 $\text{median}(\text{fc}) = -0.6641$ $\text{sd}(\text{fc}) = 1.1804$

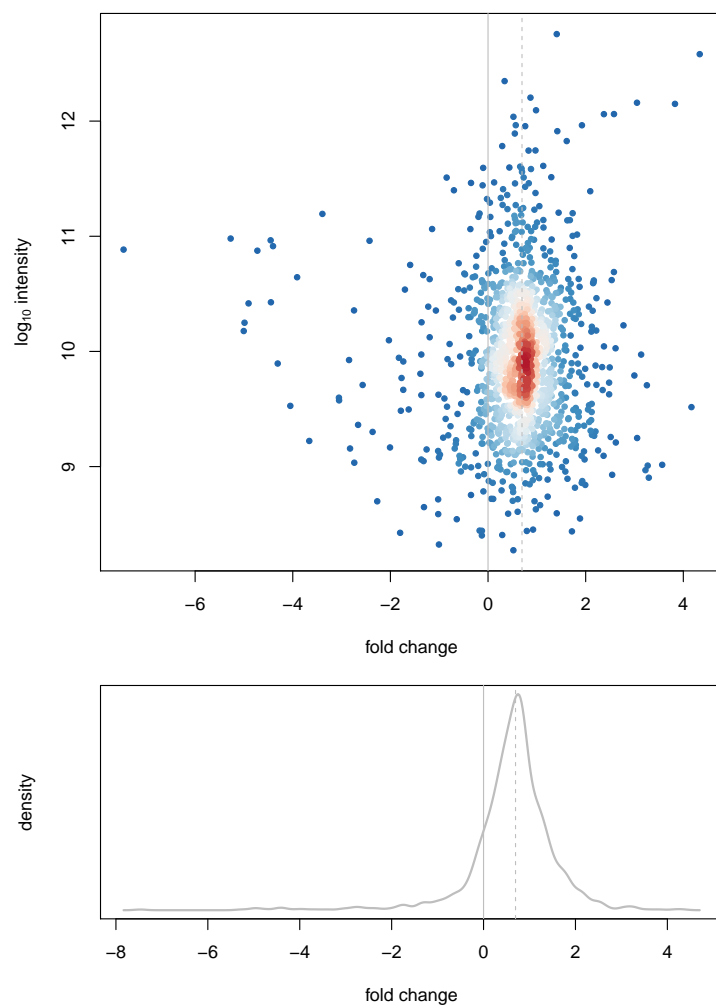


Figure 7: Fold changes of peptide abundances 2 and 3.
 $\text{median}(\text{fc}) = 0.6958$ $\text{sd}(\text{fc}) = 0.9636$

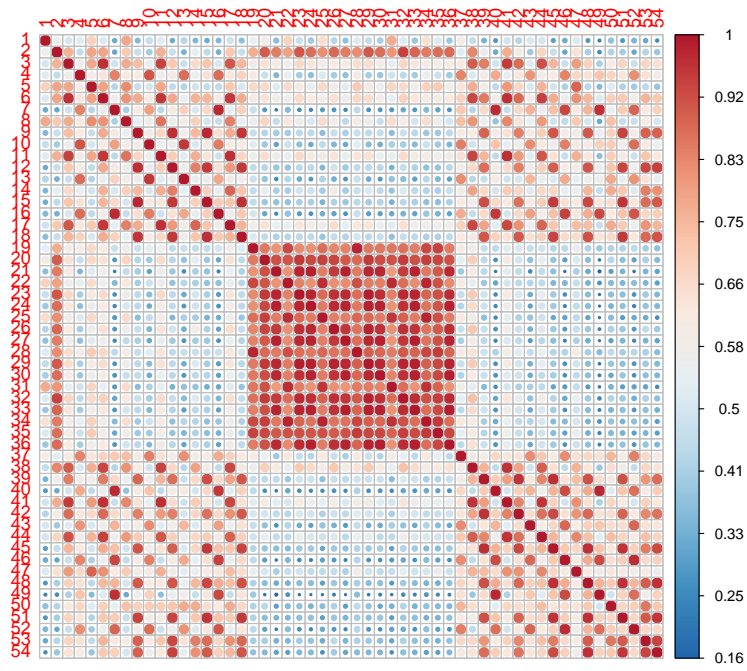


Figure 8: Pearson correlation of all peptide abundances. (min correlation = 0.1622, median correlation = 0.5936, max correlation = 1)

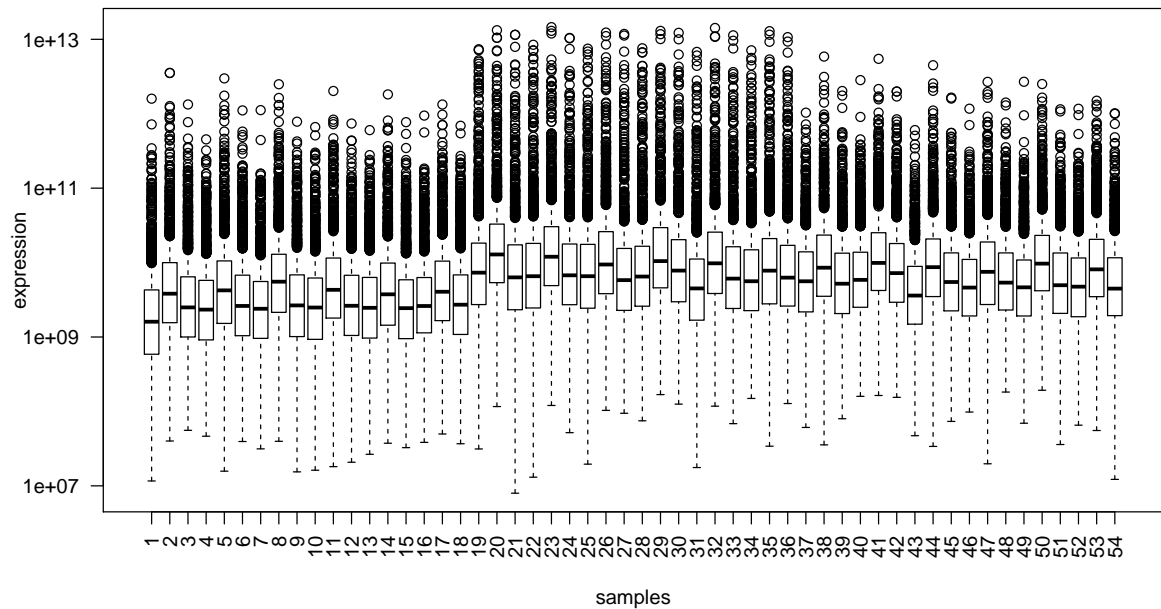


Figure 9: Boxplot of all peptide abundances.

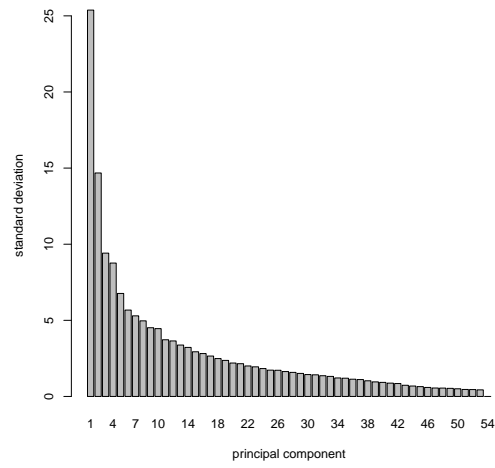


Figure 10: PCA components.

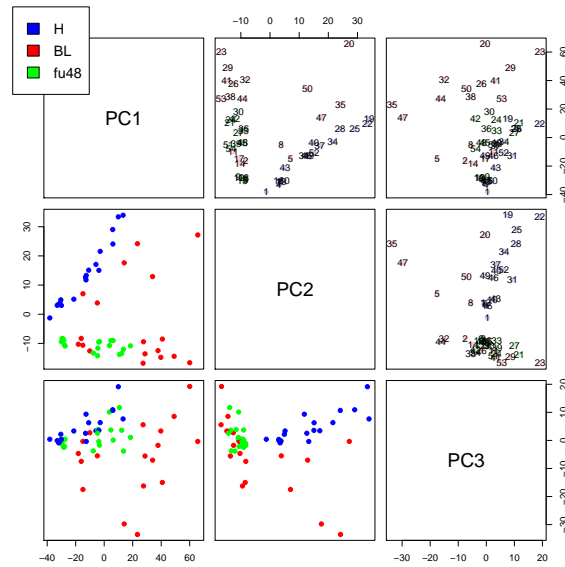


Figure 11: Principal Component Analysis of all peptides with complete quantifications. Any peptides with one or more missing values are ignored. The numbers in the upper right panels correspond to the sample IDs.

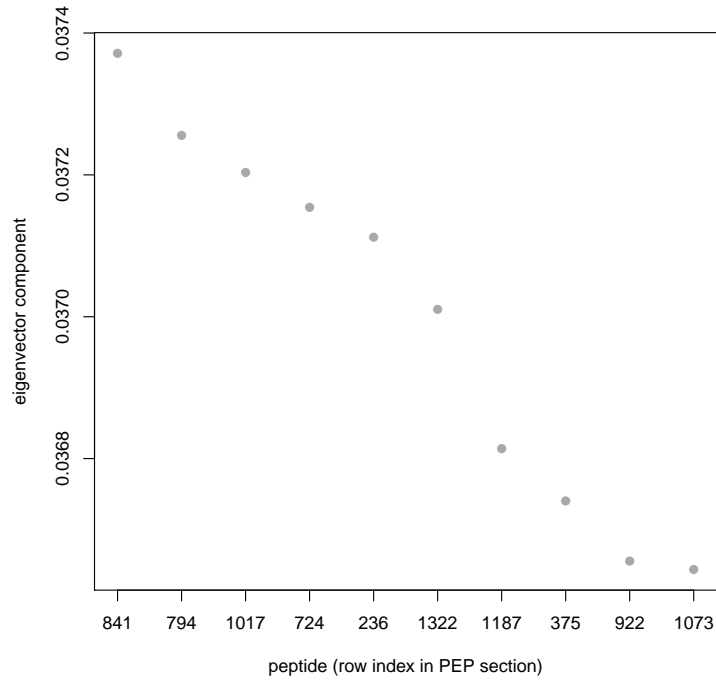


Figure 12: PCA 1st eigenvector.

modified sequence	accession	charge	retention time	m/z
LVPFDHAESTYGLYR	O95336	3	6753.43	589.96
TTPPVLDSDGSFFLYSK	P01857	2	9523.72	937.46
VLKQVHPDTGISSK	P62807	2	1911.32	754.92
LYSILGTTTLKDEGK	O75083	2	6063.81	769.43
FLPSELRDEH	Q9Y490	2	3804.75	621.81
YGFIEGHVVIPR	P16070	3	6095.82	462.92
TPAQYDASELK	P07355	2	3190.51	611.80
TSASILR	P17987	2	3663.84	430.76
ILYSQC(Methylthio)GDVM(Ox...	P14649	2	5333.98	673.80
ERQEAEAKEALLQASR	P26038	3	4365.68	653.34

Table 3: PCA 1st eigenvector.

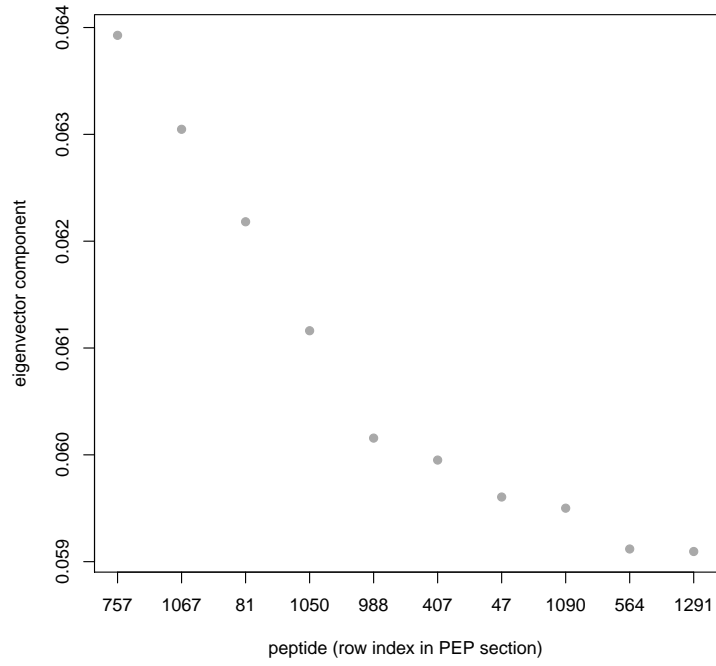


Figure 13: PCA 2nd eigenvector.

modified sequence	accession	charge	retention time	m/z
GAVDGGLSIPHSTK	P46777	2	3445.54	669.85
AIVAIENPADVSVISSR	P08865	2	8158.61	870.98
NVHGINFVSPVR	P53634	3	4626.45	446.91
SKDIVLVAYSALGSQR	P42330	3	7358.33	569.65
IAQSDYIPTQQDVL	P04899	2	6684.21	873.95
LM(Oxidation)VALAK	P07355	2	3119.97	381.23
LLDAVDTYIPVPAR	P49411	2	9218.90	771.93
TPALVNAAVTYSKPR	O75964	3	4964.94	529.97
IKIGDPLLEDTR	P49189	3	5956.77	457.26
SGDSEVYQLGDVSQK	Q04837	2	5178.78	806.38

Table 4: PCA 2nd eigenvector.

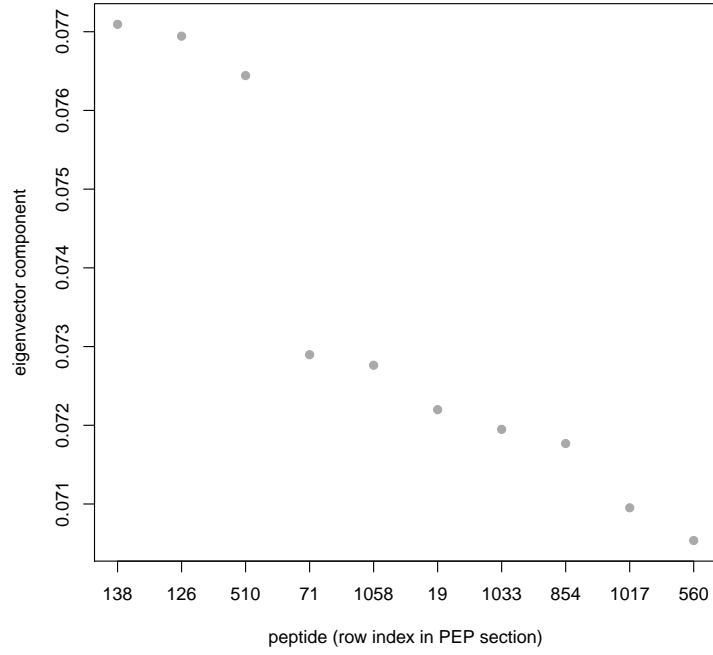


Figure 14: PCA 3rd eigenvector.

modified sequence	accession	charge	retention time	m/z
VTAPDVDLHLKAPK	Q09666	3	4409.15	501.96
KDDLGDNLHDYLR	Q9NUV9	3	5318.69	558.94
GFGFVLFK	Q14103	2	9123.27	457.76
IFVGGLSPDTPEEK	Q14103	2	6171.10	744.88
TFVNITPAEVGVLVGKDR	P07737	3	8764.50	639.03
TIISYIDEQFER	Q15019	2	9451.35	757.38
DREVGIPPEQSLETAK	P61158	2	4599.94	884.96
LAQAAQSSVATITR	Q9Y490	2	3767.92	708.89
VLKQVHPDTGISSK	P62807	2	1911.32	754.92
HIYYITGETKDQVANSADFVER	P07900	4	5448.50	611.06

Table 5: PCA 3rd eigenvector.

modified sequence	accession	charge	retention time	m/z
GNFGGSFAGSFGGAGGHAPGVAR	P52272	3	5570.46	678.99

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.

modified sequence	accession	charge	retention time	m/z
AGTQIENIDEDFRDGLK	O43707	3	6848.07	640.98
AIM(Oxidation)TYVSSFYHAFS...	O43707	3	8185.78	675.32
ALDFIASK	O43707	2	4963.37	432.74
DGLAFNALIHR	O43707	2	7035.73	613.84
ELPPDQAEYC(Methylthio)IAR	O43707	2	6999.29	775.85
ETDTDADQVIASF	O43707	2	8062.69	871.41
LSGSNPYTTVTPQIINSK	O43707	2	6625.51	960.51
LVSIGAEIIVDGNK	O43707	2	6663.17	757.91
M(Oxidation)APYQGPDAVPGAL...	O43707	2	6433.07	904.93
M(Oxidation)LDAEDIVNTARPD...	O43707	3	5738.10	611.63
M(Oxidation)LDAEDIVNTARPD...	O43707	2	5737.40	916.94
TINEVENQILTR	O43707	2	6198.35	715.39
DNHLLGTFDLTGIPPAPR	P11021	3	9502.66	645.34
IDTRNELESYAYSLK	P11021	3	6935.43	601.30
IINEPTAAAIAAYGLDK	P11021	2	8020.47	830.45
ITPSYVAFTPEGER	P11021	2	6421.94	783.89
LYGSAGPPPTGEEDTAEKDEL	P11021	2	5768.97	1088.50
NQLTSNPENTVFDAK	P11021	2	5446.82	839.41
NQLTSNPENTVFDAKR	P11021	3	4260.53	611.97
SQIFSTASDNQPTVTIK	P11021	2	6081.44	918.97
TKPYIQVDIGGGQTK	P11021	3	4136.75	535.63
TWNDPSVQQDIK	P11021	2	4695.89	715.85
VTHAVVTVPAYFNDAQR	P11021	3	5758.44	629.99
VYEGERPLTK	P11021	2	1926.05	596.32

Table 7: Proteins of interest.