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.

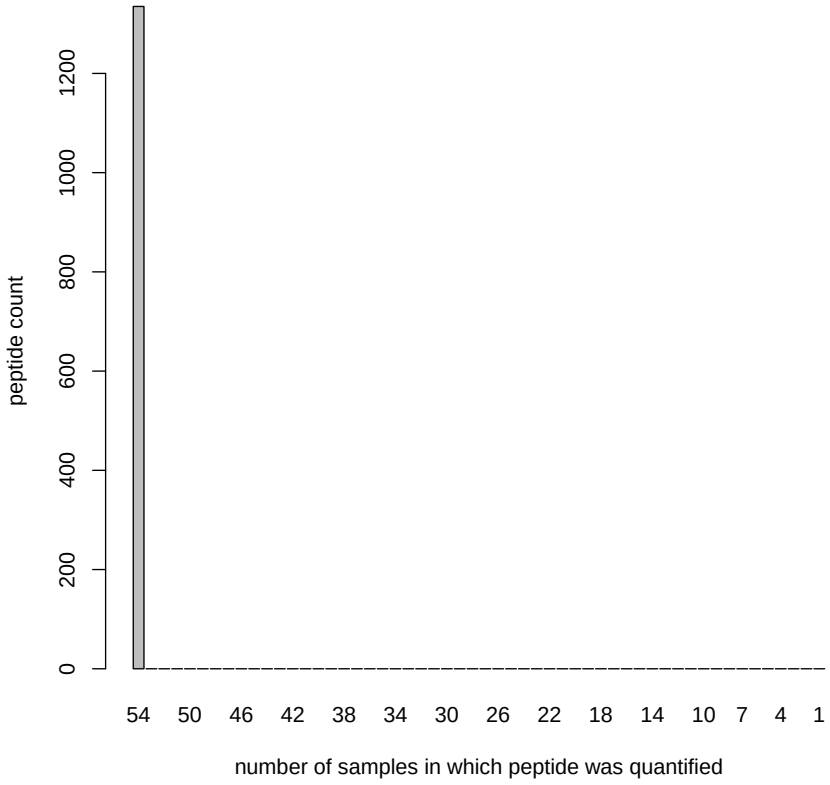


Figure 1: Frequency plot of peptide quantifications.

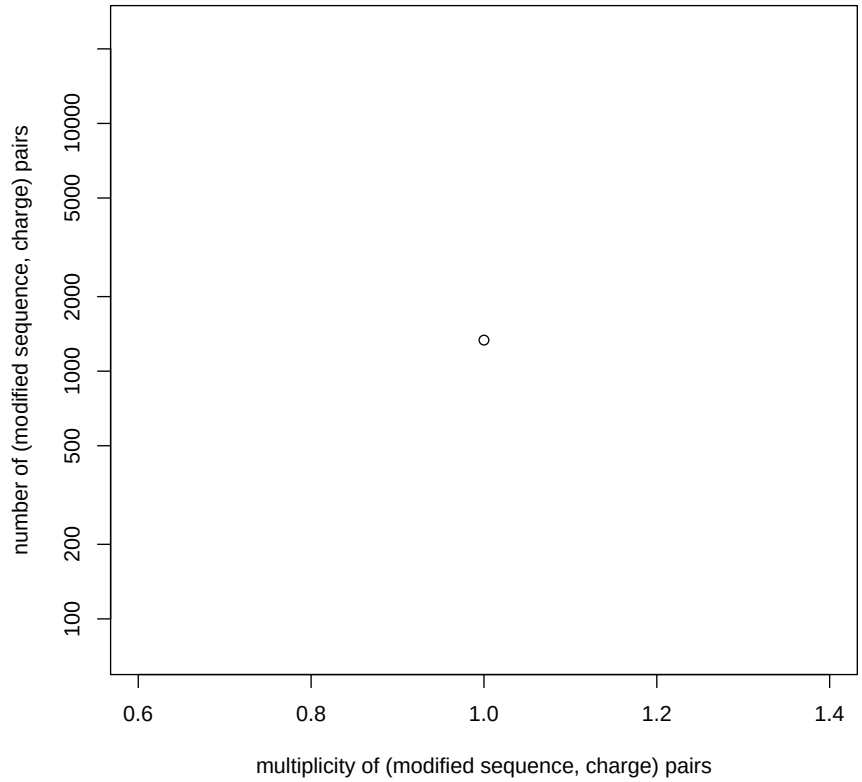
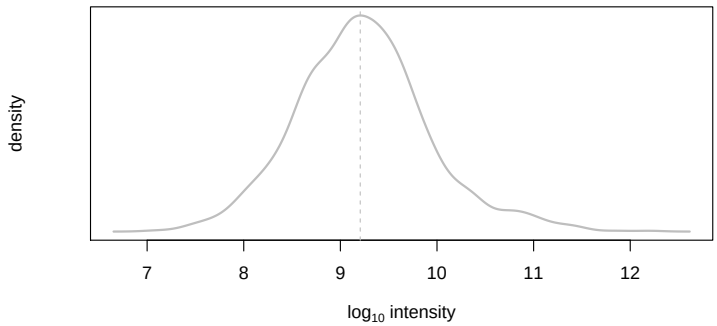
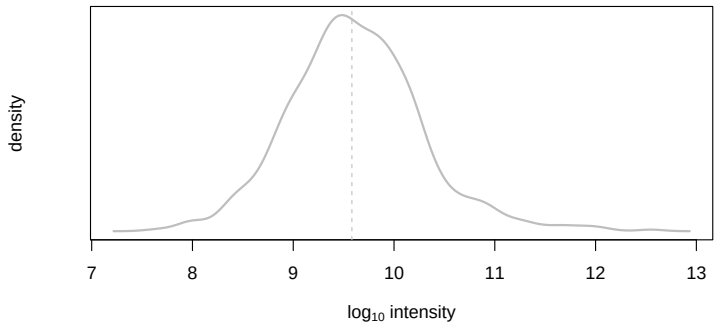


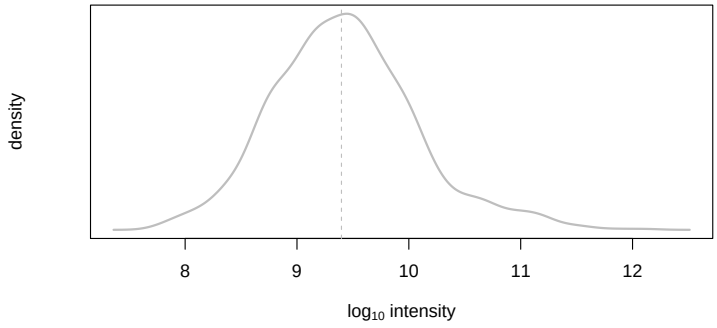
Figure 2: (modified sequence, charge) pair multiplicity vs frequency plot. Each peptide feature (characterised by a (possibly) modified peptide sequence and a charge state) should ideally occur only once in the analysis. In other words, peptides of multiplicity 1 should have a very high frequency. The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



(a) peptide abundances 1, 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 3: peptide abundance distributions.

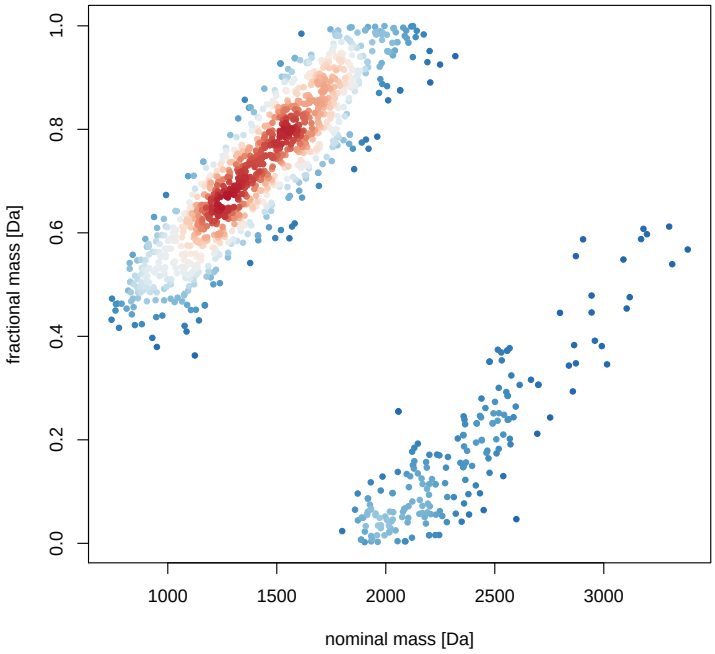


Figure 4: Kendrick nominal fractional mass plot

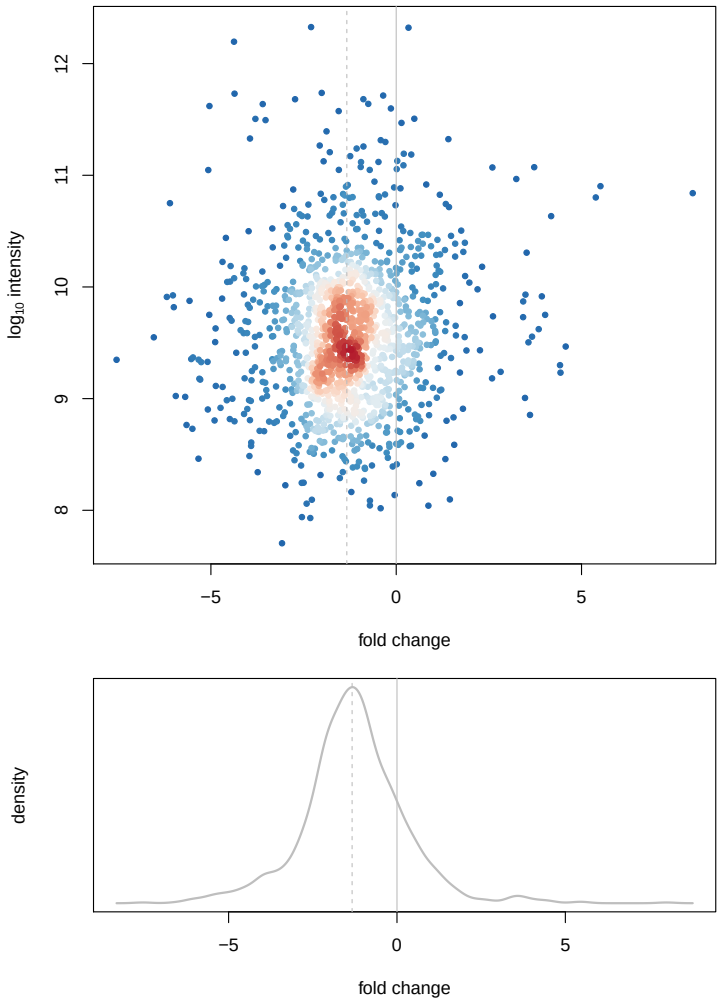


Figure 5: Fold changes of peptide abundances 1 and 2.
median(fc) = −1.3328 sd(fc) = 1.5445

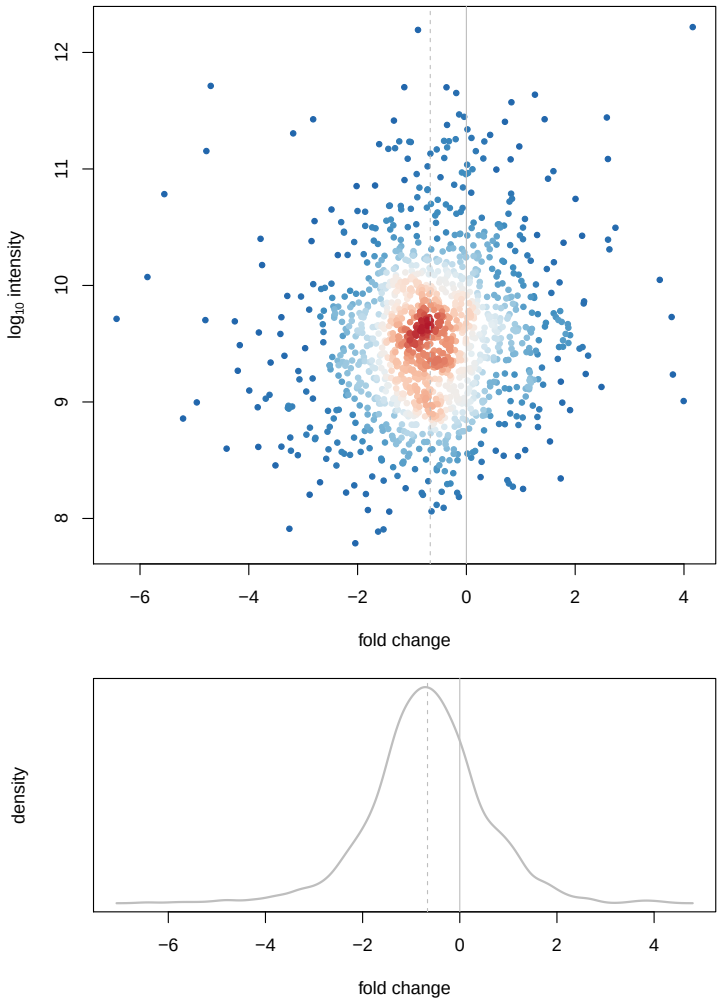


Figure 6: Fold changes of peptide abundances 1 and 3.
median(fc) = −0.6641 sd(fc) = 1.1804

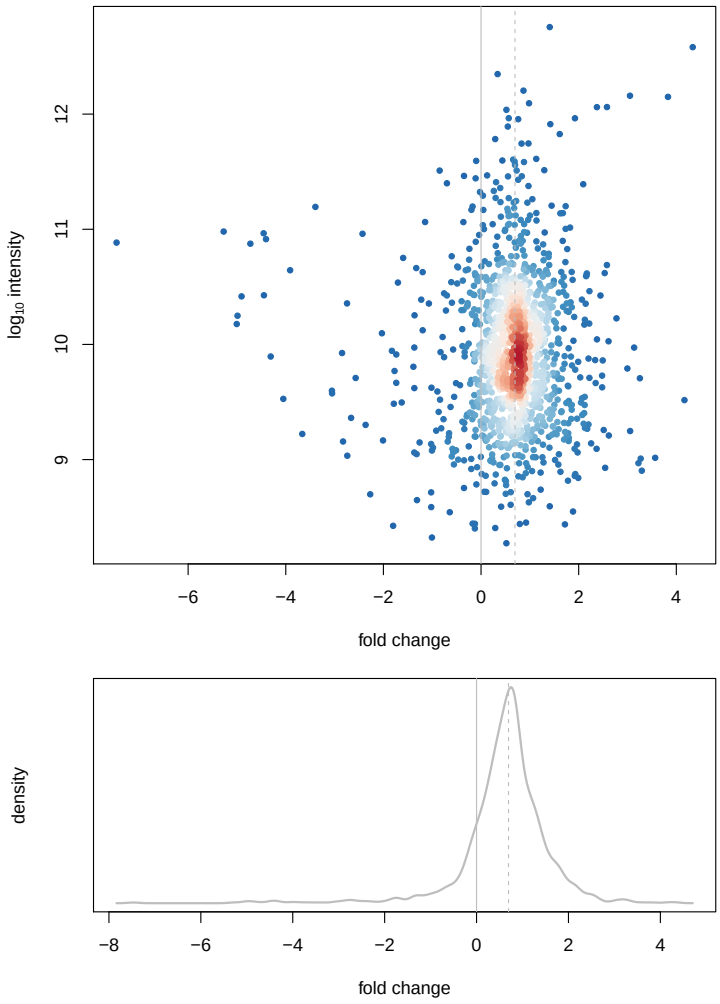


Figure 7: Fold changes of peptide abundances 2 and 3.
median(fc) = 0.6958 sd(fc) = 0.9636

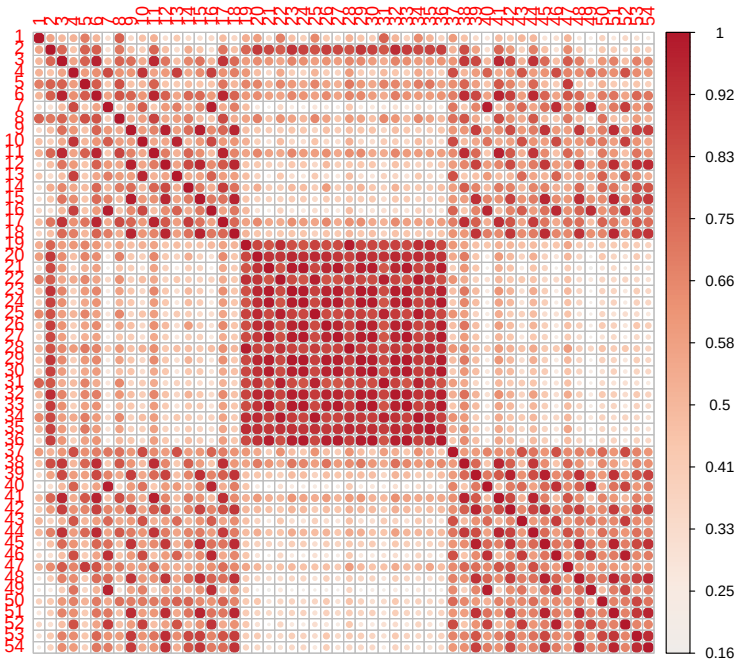


Figure 8: Pearson correlation of all peptide abundances. (min correlation = 0.1622, median correlation = 0.5936, max correlation = 1)

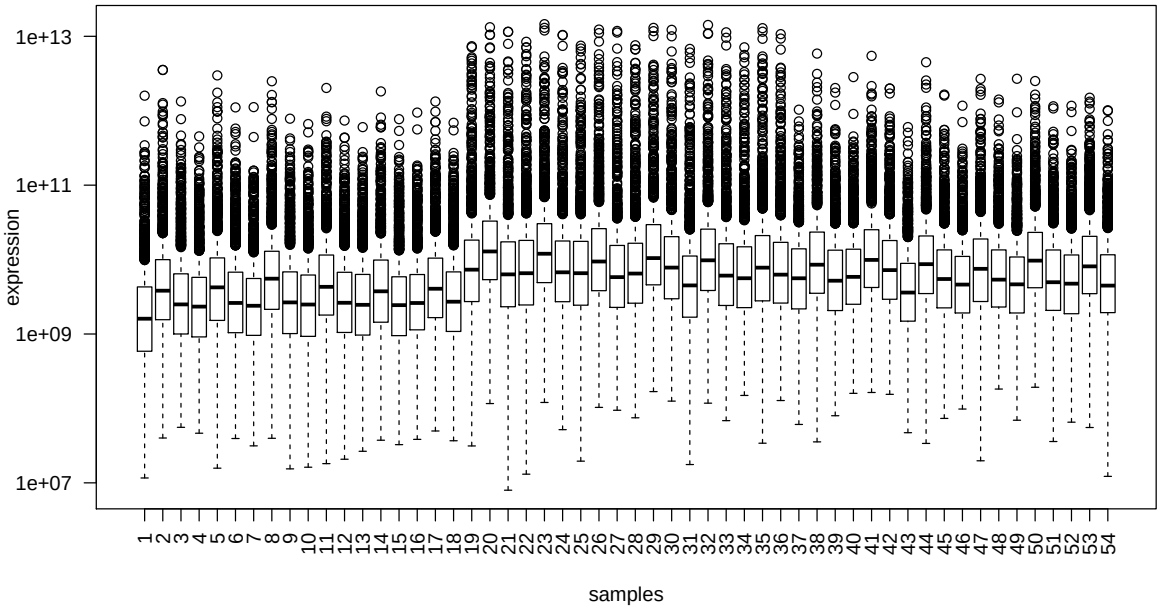


Figure 9: Boxplot of all peptide abundances.

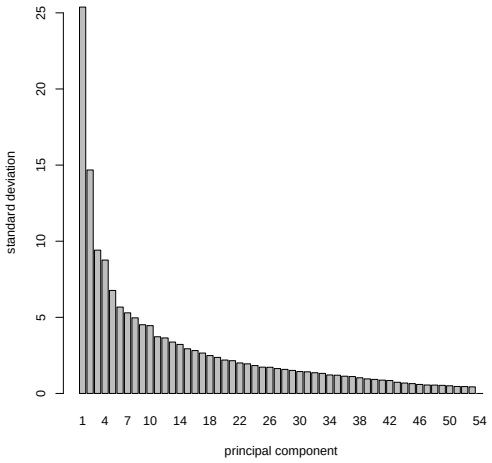


Figure 10: PCA components.

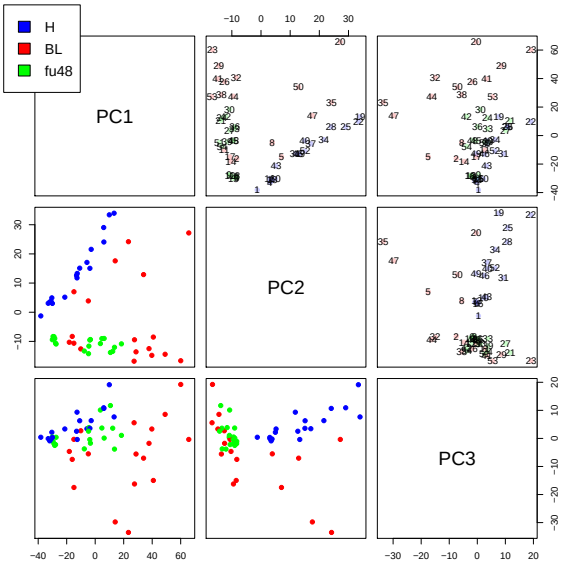


Figure 11: Principal Component Analysis of all peptides with complete quantifications. Any peptides with one or more missing values are ignored. The numbers in the upper right panels correspond to the sample IDs.

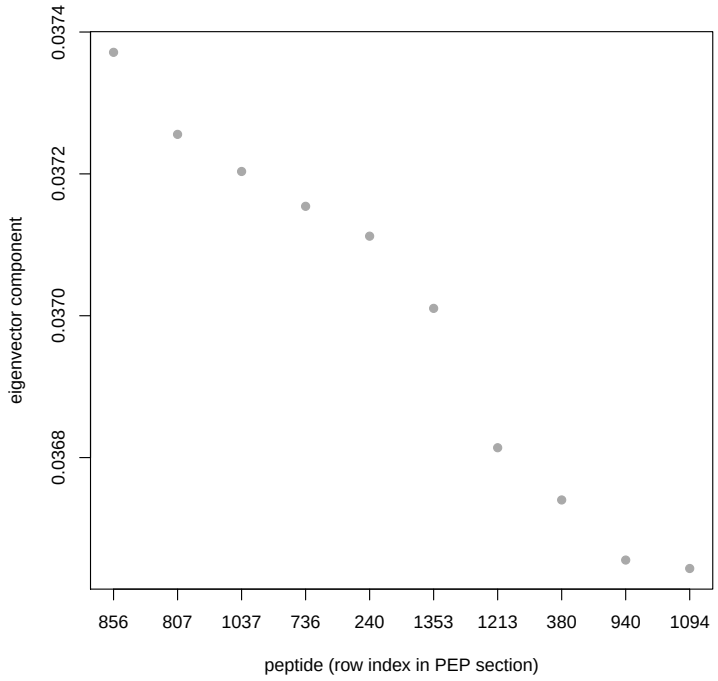


Figure 12: PCA 1st eigenvector.

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	TSASIILR	P17987	2	3663.84	430.76
940	ILYSQC(Methylthio)GDVM(Ox...	P14649	2	5333.98	673.80
1094	ERQEAEEAKEALLQASR	P26038	3	4365.68	653.34

Table 3: PCA 1st eigenvector.

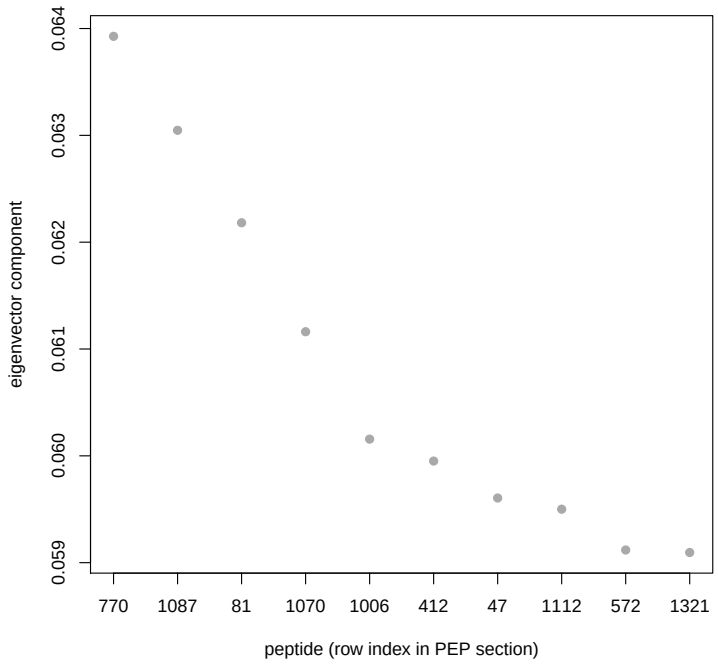


Figure 13: PCA 2nd eigenvector.

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	IAQSDYIPTQQDVLR	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: PCA 2nd eigenvector.

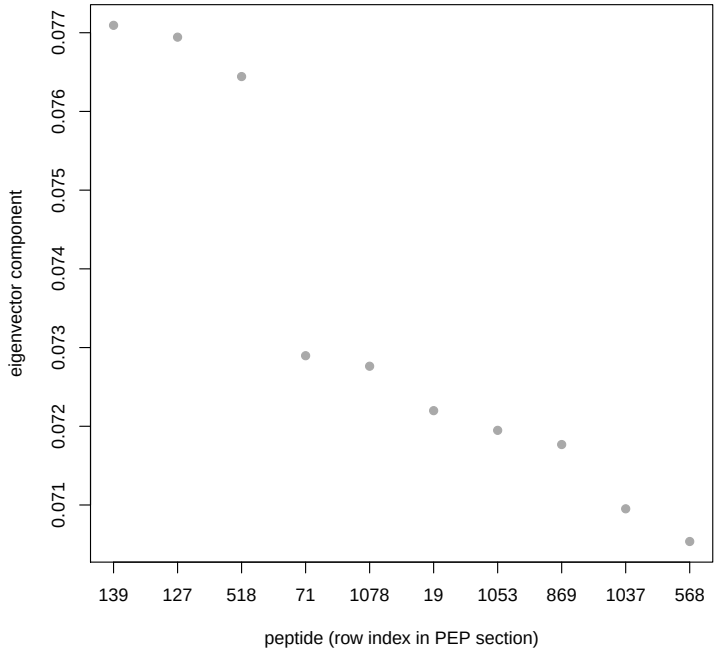


Figure 14: PCA 3rd eigenvector.

row index	modified sequence	accession	charge	retention time	m/z
139	VTAPDVDLHLKAPK	Q09666	3	4409.15	501.96
127	KDDLGDTNLHDYLR	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	HIYYITGETKDQVANSAFVER	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
ETTDTDTADQVIASFK	O43707	2	8062.69	871.41
LSGSNPYTTVTPQIINSK	O43707	2	6625.51	960.51
LVSIGAEEIVDGNAK	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
IINEPTAAAIAYGLDK	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.