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.

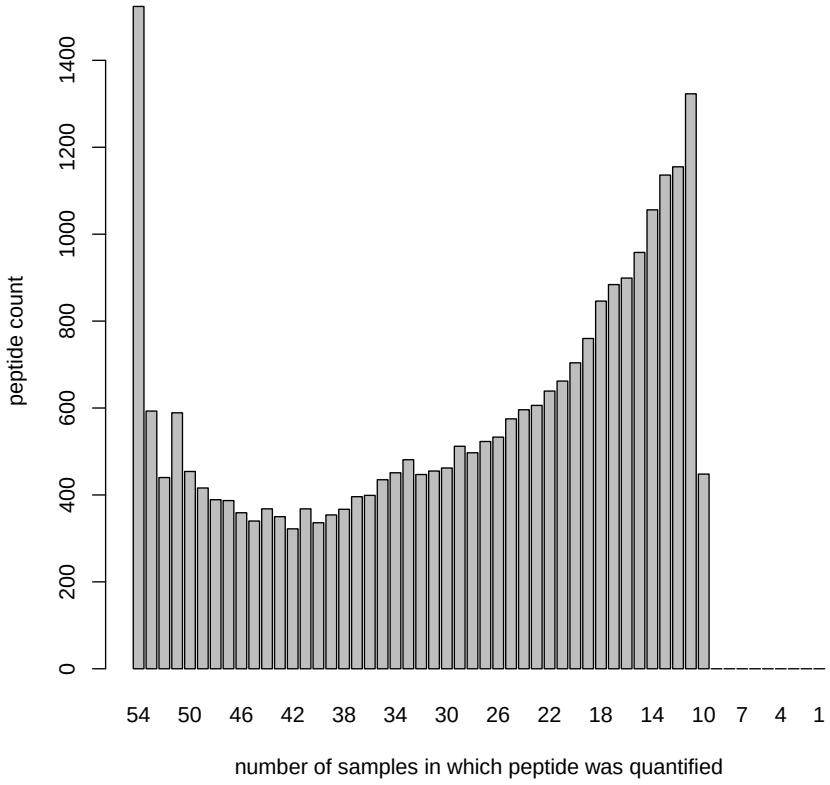


Figure 1: Frequency plot of peptide quantifications.

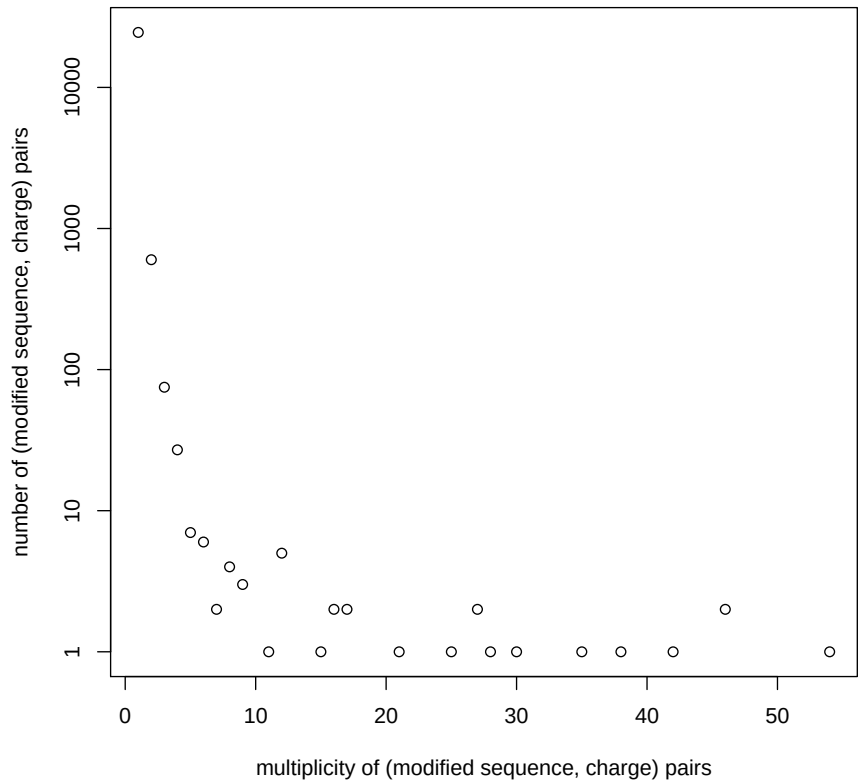
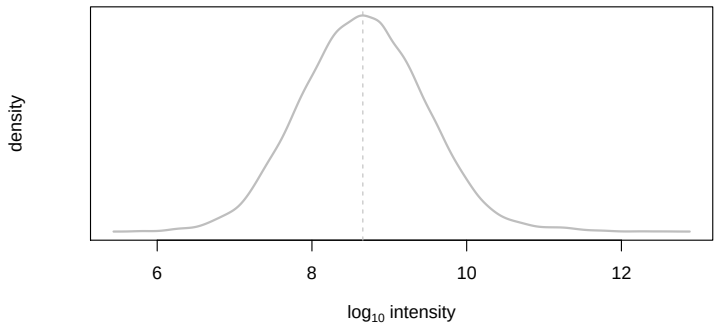
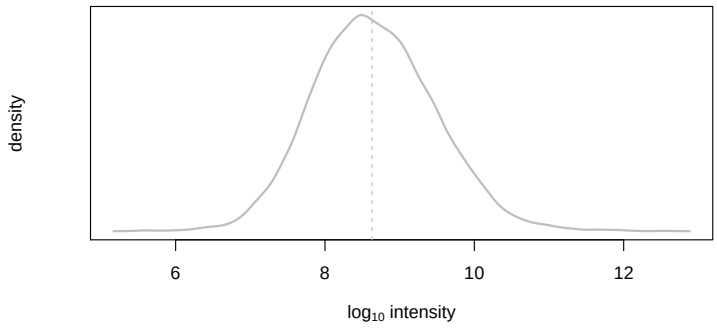


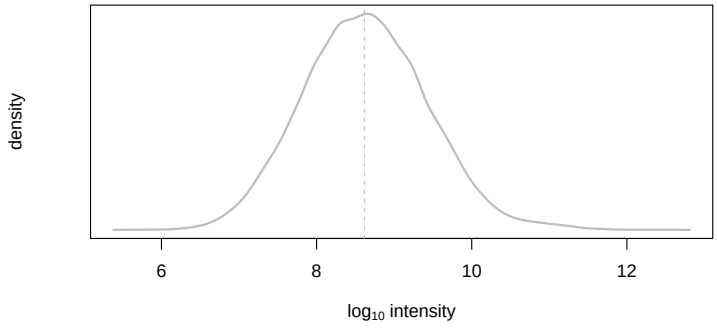
Figure 2: (modified sequence, charge) pair multiplicity vs frequency plot. Each peptide feature (characterised by a (possibly) modified peptide sequence and a charge state) should ideally occur only once in the analysis. In other words, peptides of multiplicity 1 should have a very high frequency. The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



(a) peptide abundances 1, median(intensity) = $455,025,504$



(b) peptide abundances 2, median(intensity) = $424,578,000$



(c) peptide abundances 3, median(intensity) = $412,578,512$

Figure 3: peptide abundance distributions.

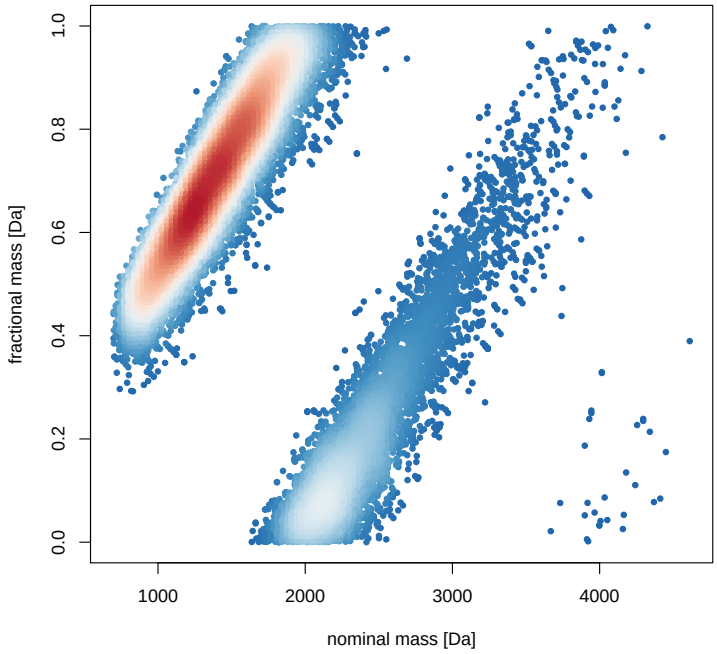


Figure 4: Kendrick nominal fractional mass plot

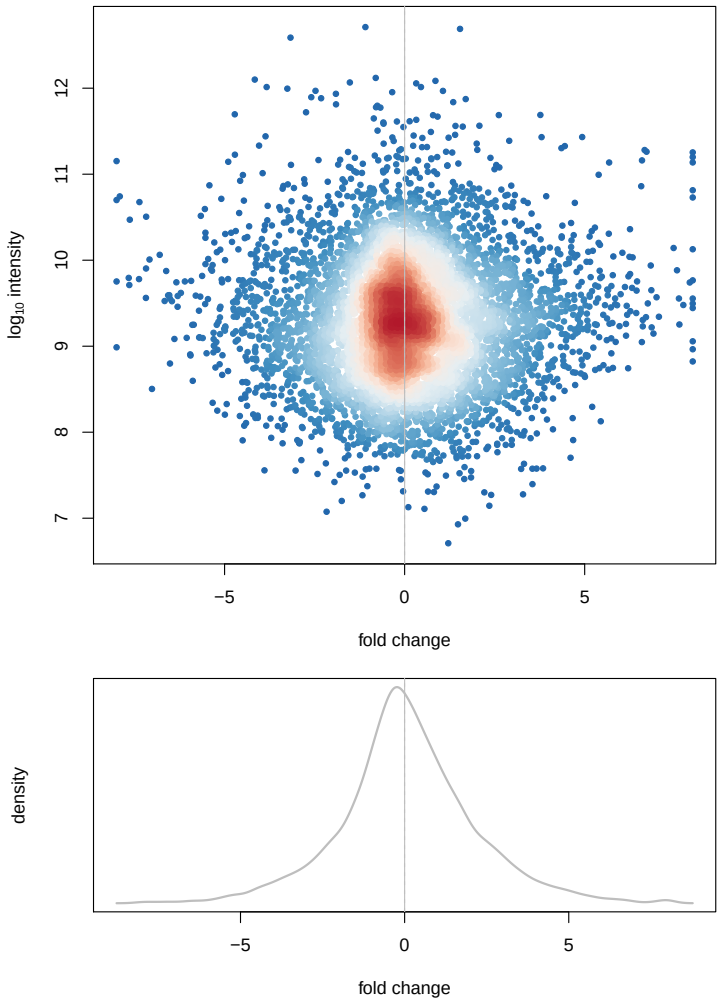


Figure 5: Fold changes of peptide abundances 1 and 2.
median(fc) = −0.0026 sd(fc) = 2.0776

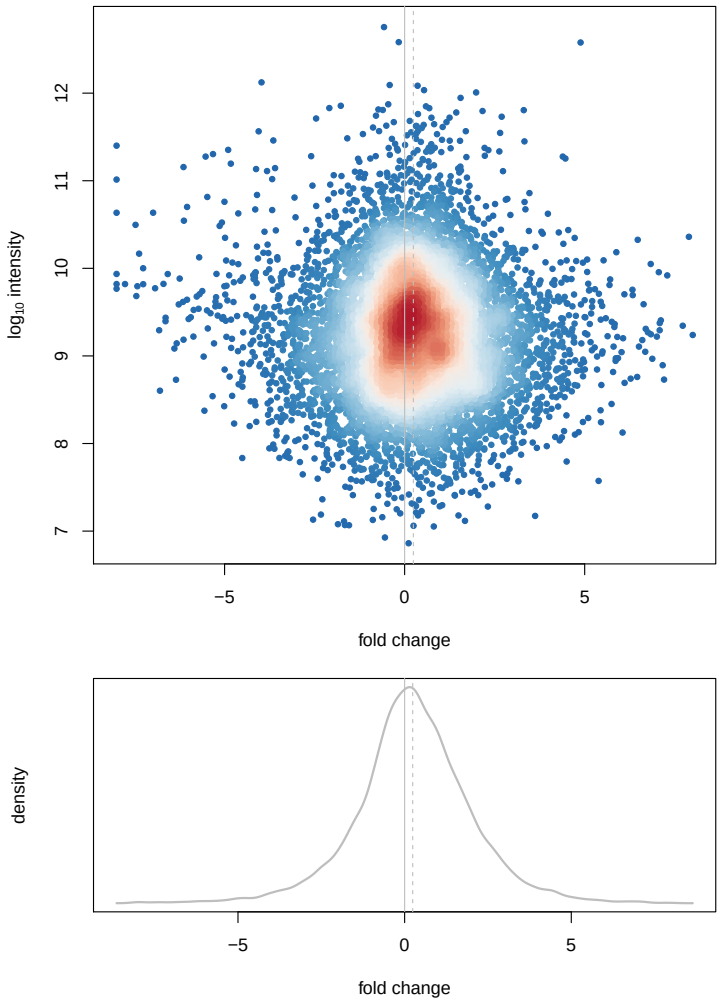


Figure 6: Fold changes of peptide abundances 1 and 3.
median(fc) = 0.2421 sd(fc) = 1.7661

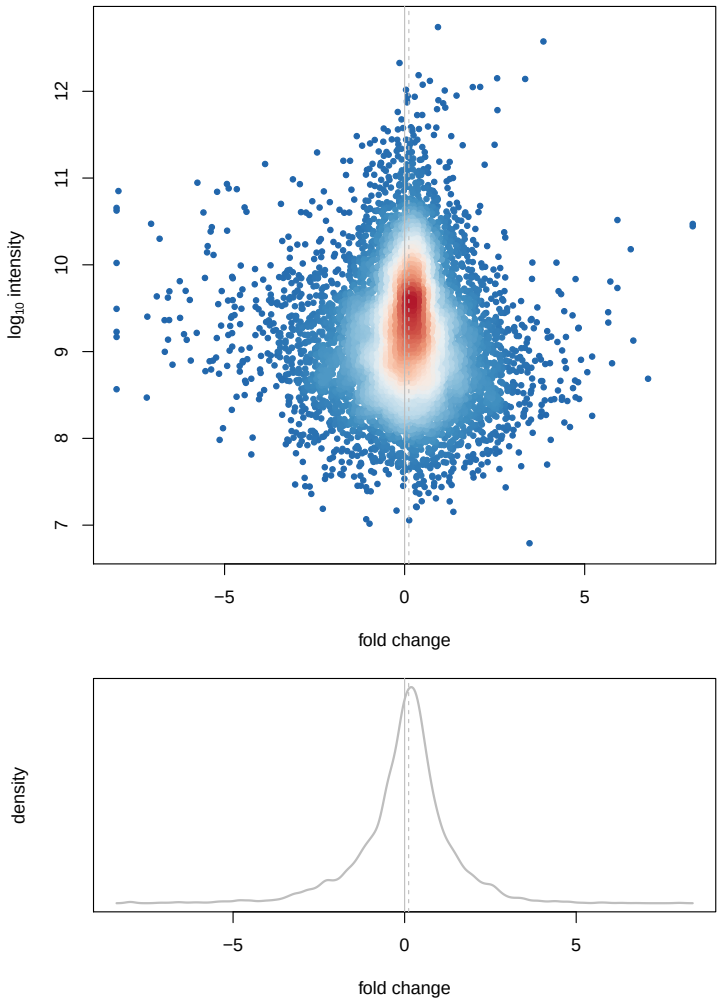


Figure 7: Fold changes of peptide abundances 2 and 3.
median(fc) = 0.1175 sd(fc) = 1.3543

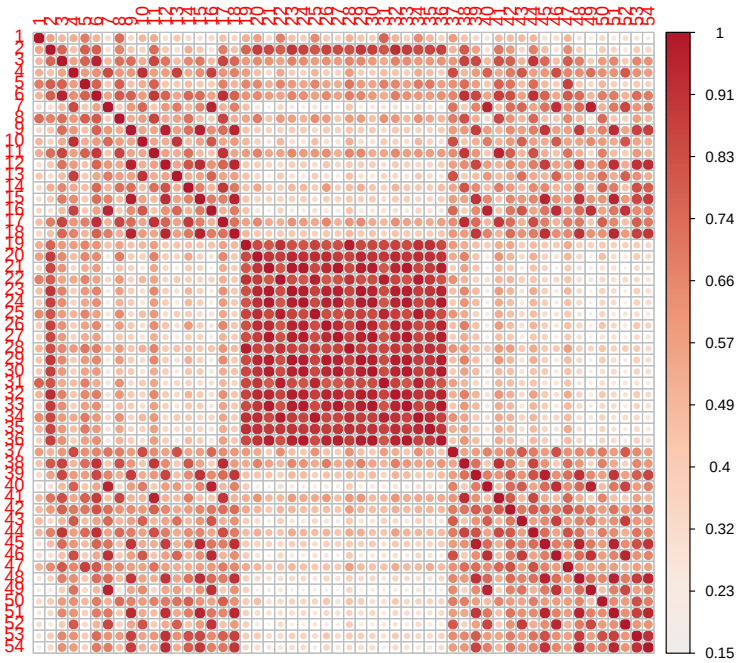


Figure 8: Pearson correlation of all peptide abundances. (min correlation = 0.1484, median correlation = 0.5701, max correlation = 1)

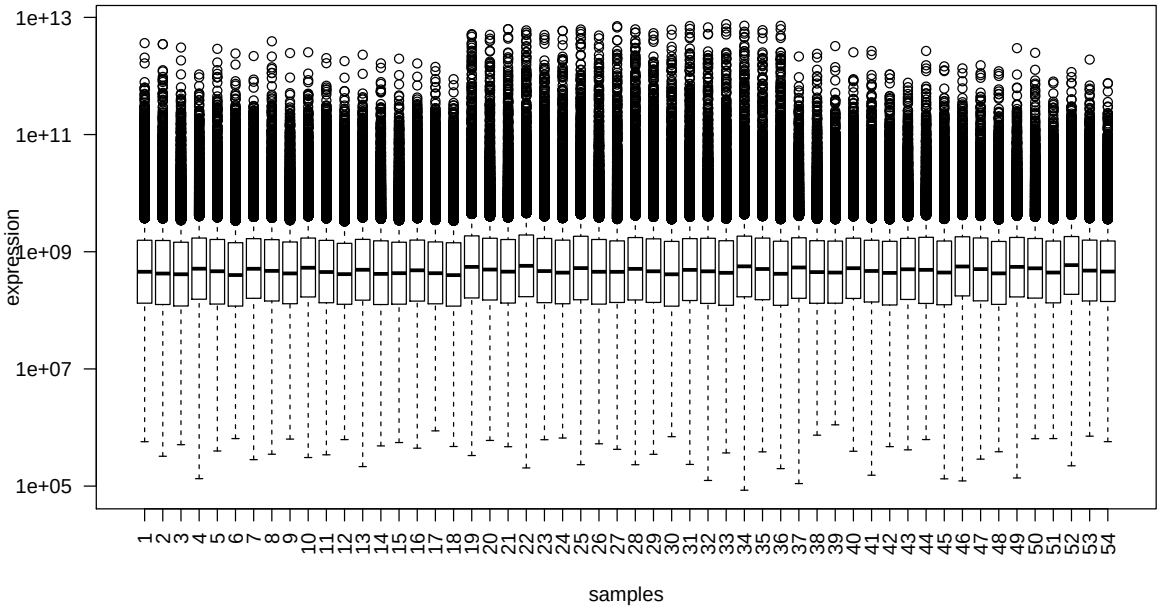


Figure 9: Boxplot of all peptide abundances.

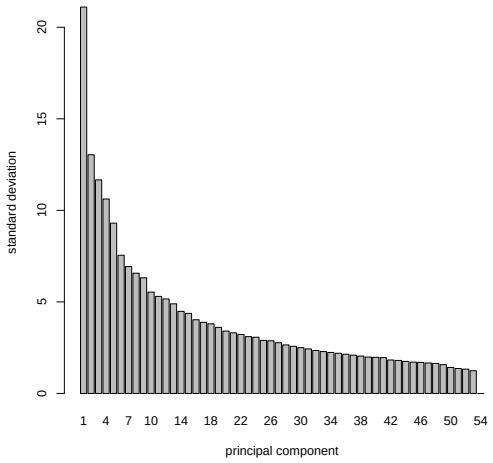


Figure 10: PCA components.

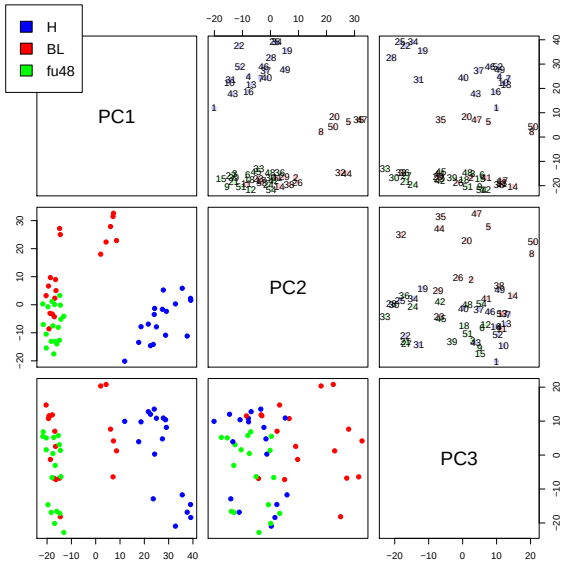


Figure 11: Principal Component Analysis of all peptides with complete quantifications. Any peptides with one or more missing values are ignored. The numbers in the upper right panels correspond to the sample IDs.

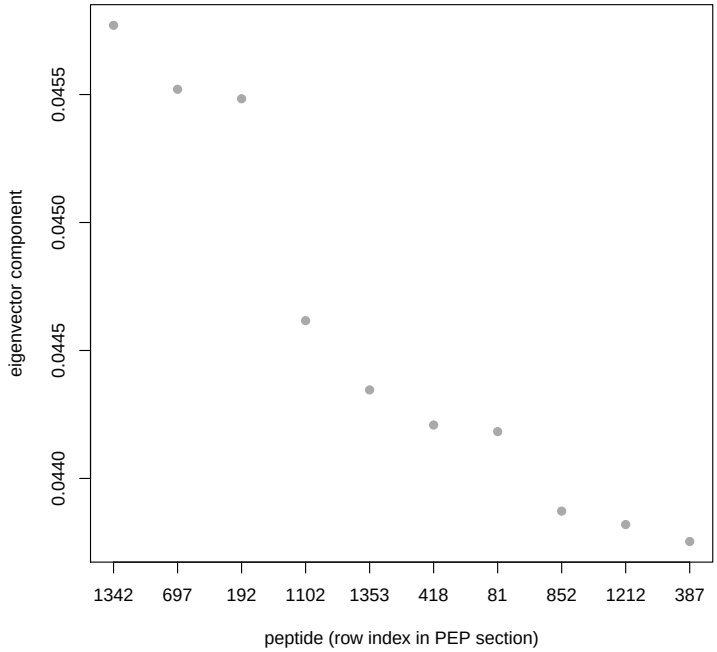


Figure 12: PCA 1st eigenvector.

row index	modified sequence	accession	charge	retention time	m/z
1342	IVAPGKGILAADESTGSIAK	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	TIIPLISQC(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: PCA 1st eigenvector.

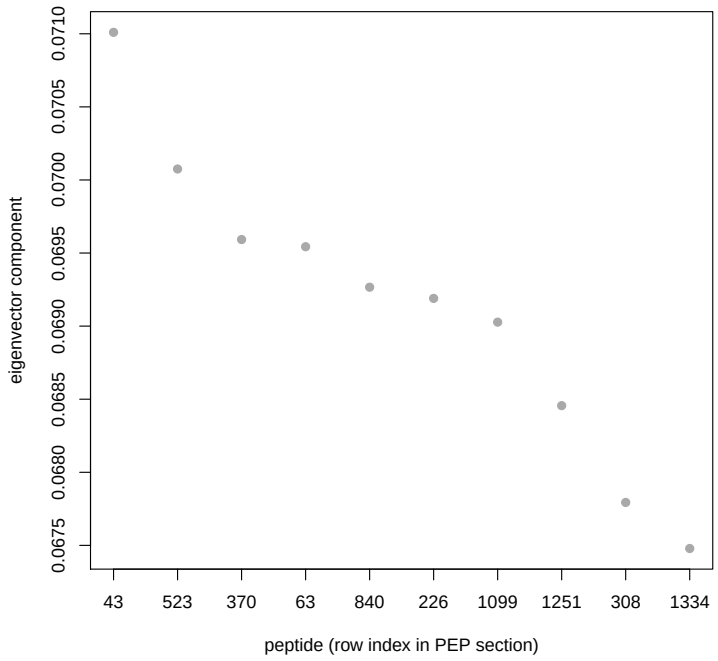


Figure 13: PCA 2nd eigenvector.

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: PCA 2nd eigenvector.

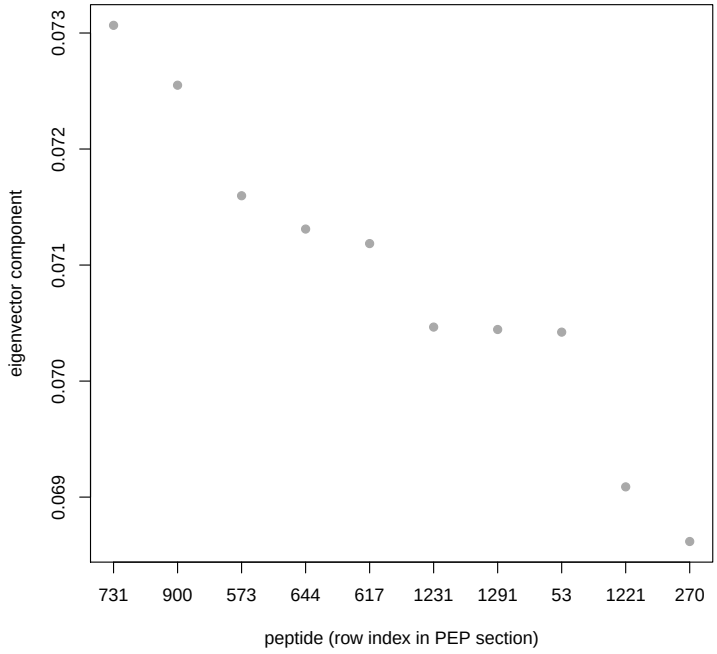


Figure 14: PCA 3rd eigenvector.

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	VALVYGQMNEPPGAR	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	AVEVQGPSLESGDHGK	Q09666	3	2851.80	537.27

Table 5: PCA 3rd eigenvector.

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
TVPFC(Methylthio)STFAAFFT...	P29401	2	12736.46	820.88
GNFGGSFAGSFGGAGGHAPGVAR	P52272	3	5570.46	678.99
GNFGGSFAGSFGGAGGHAPGVAR	P52272	2	5569.35	1017.98
GNFGGSFAGSFGGAGGHAPGVARK	P52272	4	4336.39	541.52
GNFGGSFAGSFGGAGGHAPGVARK	P52272	3	4346.43	721.69

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
AC(Methylthio)LISLGYDVEND...	O43707	3	8518.39	849.05
AGTQIENIDEDFRDGLK	O43707	3	6848.07	640.98
AGTQIENIDEDFRDGLK	O43707	2	6847.12	960.97
AIM(Oxidation)TYVSSFYHAFS...	O43707	3	8185.69	675.32
AIM(Oxidation)TYVSSFYHAFS...	O43707	2	8172.79	1012.48
AIMTYVSSFYHAFSGAQK	O43707	3	9592.08	669.99
AIMTYVSSFYHAFSGAQK	O43707	2	9597.33	1004.49
AIM(Oxidation)TYVSSFYHAFS...	O43707	3	9596.21	675.32
AIM(Oxidation)TYVSSFYHAFS...	O43707	4	7575.23	685.08
AIM(Oxidation)TYVSSFYHAFS...	O43707	3	7571.39	913.11
AIMTYVSSFYHAFSGAQKAETAANR	O43707	3	8754.95	907.77
ALDFIASK	O43707	2	4963.37	432.74
ASFNHFDKDHGGALGPEEFK	O43707	4	4122.09	551.51
ASFNHFDKDHGGALGPEEFK	O43707	3	4144.77	735.01
ASIHEAWTDGKEAM(Oxidation)...	O43707	3	3348.57	601.63
ASIHEAWTDGKEAM(Oxidation)...	O43707	4	3349.63	451.47
ASIHEAWTDGKEAMLK	O43707	3	4519.42	596.30
ASIHEAWTDGKEAMLK	O43707	4	4527.79	447.47
C(Methylthio)QLEINFNTLQTK	O43707	2	8884.72	799.39
DAKGISQEQM(Oxidation)QEFR	O43707	3	2737.85	561.60
DAKGISQEQM(Oxidation)QEFR	O43707	2	2742.44	841.89
DDPVTNLNNAFEVAEK	O43707	2	9082.35	888.43
DDPVTNLNNAFEVAEKYLDIPK	O43707	3	12761.98	835.76
DGLAFNALIHR	O43707	2	7035.73	613.84
DGLAFNALIHR	O43707	3	7033.86	409.56
DYETATLSDIK	O43707	2	6094.41	628.31
EAILAIHK	O43707	2	2743.24	447.77
EAILAIHKEAQR	O43707	3	2210.93	460.26
EAILAIHKEAQR	O43707	2	2215.06	689.89
EALEKTEKQLEAIDQLHLEYAK	O43707	4	7225.32	650.60
EGLLLWC(Methylthio)QR	O43707	2	9692.16	582.29
ELPPDQAEYC(Methylthio)IAR	O43707	2	7002.71	775.85
ELPPDQAEYC(Methylthio)IAR	O43707	2	7083.91	775.85
ETTDTDTADQVIASFK	O43707	2	8062.69	871.41

FAIQDISVEETSAK	O43707	2	7063.20	769.39
GISQEQM(Oxidation)QEFR	O43707	2	2739.50	684.81
GISQEQMQEFR	O43707	2	4339.88	676.82
GISQEQM(Oxidation)QEFR	O43707	2	4353.66	684.81
GYEEWLLNEIR	O43707	2	10169.93	711.36
HRDYETATLSDIK	O43707	3	3041.19	516.93
HRPELIEYDK	O43707	3	2334.19	433.89
HRPELIEYDK	O43707	2	2317.06	650.34
HRPELIEYDKLR	O43707	4	3072.91	392.97
HRPELIEYDKLR	O43707	3	3056.43	523.62
HRPELIEYDKLRK	O43707	4	2437.01	424.99
HTNYTMEHIR	O43707	2	1866.52	651.30
HTNYTM(Oxidation)EHIR	O43707	3	1455.93	439.87
HTNYTM(Oxidation)EHIR	O43707	2	1456.59	659.30
HTNYTMEHIR	O43707	3	1855.45	434.54
IAESNHIK	O43707	2	1235.63	456.25
IAESNHIKLSGSNPYTTVTPQIINS...	O43707	4	5891.40	703.88
IC(Methylthio)DQWDALGSLTH...	O43707	3	8717.28	583.27
INNVNKALDFIASK	O43707	3	6288.21	516.29
ISIEMNGTLEDQLSHLK	O43707	3	8458.92	643.33
ISIEM(Oxidation)NGTLEDQLS...	O43707	3	7310.00	648.66
ISIEM(Oxidation)NGTLEDQLS...	O43707	4	7457.52	630.82
KAGTQIENIDEDFRDGLK	O43707	3	5572.19	683.68
KAGTQIENIDEDFRDGLK	O43707	4	5566.69	513.01
KDDPVTNLNNAFEVAEK	O43707	3	6826.99	635.32
KDDPVTNLNNAFEVAEK	O43707	2	6826.29	952.47
KDDPVTNLNNAFEVAEKYLDIPK	O43707	3	11618.90	878.45
KDDPVTNLNNAFEVAEKYLDIPK	O43707	4	11629.73	659.09
KTFTAWC(Methylthio)NSHLR	O43707	3	4628.27	503.91
KTFTAWC(Methylthio)NSHLRK	O43707	3	3352.06	546.61
LASDLLEWIR	O43707	2	10366.11	608.34
LASDLLEWIRR	O43707	3	8660.76	457.93
LDHLAEK	O43707	2	1399.43	413.23
LDHLAEKFR	O43707	3	2308.99	376.88
LM(Oxidation)LLLEVISGERLP...	O43707	4	8470.91	528.06
LMLLLEVISGERLPKPER	O43707	4	9520.17	524.06
LRKDDPVTNLNNAFEVAEK	O43707	4	5943.50	544.04
LRKDDPVTNLNNAFEVAEKYLDIPK	O43707	4	10641.49	726.39
LSGSNPYTTVTPQIINSK	O43707	2	6625.51	960.51
LSGSNPYTTVTPQIINSKWEK	O43707	3	6923.35	788.41
LSNRPAFMPSEGK	O43707	3	3100.77	478.58
LVSIGAEEIVDGNAK	O43707	2	6663.17	757.91
M(Oxidation)APYQGPDAVPGAL...	O43707	2	6433.07	904.93
MAPYQGPDAVPGALDYK	O43707	2	7001.32	896.93
M(Oxidation)APYQGPDAVPGAL...	O43707	2	6998.59	904.93
M(Oxidation)LDAEDIVNTARPD...	O43707	3	5738.10	611.63
M(Oxidation)LDAEDIVNTARPD...	O43707	2	5737.40	916.94
MLDAEDIVNTARPDEK	O43707	3	6487.18	606.30
MLDAEDIVNTARPDEK	O43707	2	6486.87	908.94
M(Oxidation)LDAEDIVNTARPD...	O43707	3	6486.32	611.63
M(Oxidation)LDAEDIVNTARPD...	O43707	2	6492.91	916.94
NVNVQNFHISWK	O43707	2	6305.44	743.38
NVNVQNFHISWK	O43707	3	6296.92	495.92
QFASQANVVGPWIQTK	O43707	2	7605.79	887.47
QLEAIDQLHLEYAK	O43707	3	6835.31	557.63
QLEAIDQLHLEYAKR	O43707	4	5640.68	457.50

RDHALLEEQSK	O43707	3	1618.19	442.56
RDHALLEEQSKQQSNEHLR	O43707	4	1829.30	580.30
RQFASQANVVGPWIQTK	O43707	3	5919.51	644.01
RTIPWLEDRVPQK	O43707	3	4602.85	546.64
SIVDYKPNLDLLEQQHQLIQEALIF...	O43707	4	11309.39	831.94
SIVDYKPNLDLLEQQHQLIQEALIF...	O43707	3	11306.86	1108.92
TAPYKNVNVQNFHISWK	O43707	4	5925.81	512.27
TAPYKNVNVQNFHISWK	O43707	3	5922.83	682.69
TEKQLEAIDQLHLEYAK	O43707	4	5985.63	508.02
TEKQLEAIDQLHLEYAK	O43707	3	5989.08	677.02
TFTAWC(Methylthio)NSHLR	O43707	3	6199.54	461.21
TFTAWC(Methylthio)NSHLR	O43707	2	6243.15	691.31
TINEVENQILTR	O43707	2	6198.35	715.39
TIQEMQQK	O43707	2	1659.65	503.26
VGWEQLLTTIAR	O43707	2	11063.02	693.89
VHKPPKVQEK	O43707	3	1081.02	397.24
VHKPPKVQEK	O43707	2	1104.93	595.36
VLAGDKNFITAEELR	O43707	3	5870.35	559.31
VLAGDKNFITAEELR	O43707	2	5867.80	838.45
VLAGDKNFITAEELRR	O43707	4	4742.17	458.76
VLAVNQENEHLM(Oxidation)ED...	O43707	3	4114.35	692.99
VLAVNQENEHLMEDYEK	O43707	3	5428.68	687.66
VLAVNQENEHLM(Oxidation)ED...	O43707	2	4120.65	1038.98
VQQLVPK	O43707	2	2270.17	406.26
AKFEELNMDLFR	P11021	3	7827.10	504.92
AKFEELNM(Oxidation)DLFR	P11021	3	6340.88	510.25
AKFEELNM(Oxidation)DLFR	P11021	2	6341.70	764.88
AKFEELNMDLFR	P11021	2	7827.76	756.88
AVEEKIEWLESHQDADIEDFK	P11021	3	7623.84	844.40
AVEEKIEWLESHQDADIEDFKAK	P11021	4	6832.87	683.33
DAGTIAGLNVM(Oxidation)R	P11021	2	5466.52	617.32
DAGTIAGLNVMR	P11021	2	7130.61	609.32
DAGTIAGLNVM(Oxidation)R	P11021	2	7157.32	617.32
DAGTIAGLNVM(Oxidation)R	P11021	2	5517.68	617.31
DNHLLGTFDLTGIPPAPR	P11021	3	9496.78	645.34
DNHLLGTFDLTGIPPAPR	P11021	2	9506.43	967.51
DNHLLGTFDLTGIPPAPR	P11021	3	9504.56	645.34
ELEEIVQPIISK	P11021	2	7934.60	699.40
FEELNM(Oxidation)DLFR	P11021	2	7569.60	665.31
FEELNMDLFR	P11021	2	9376.14	657.31
FLPFKVVEK	P11021	2	5178.59	553.83
FLPFKVVEKK	P11021	3	3612.48	412.26
FLPFKVVEKK	P11021	2	3627.05	617.88
IDTRNELESYAYSLK	P11021	3	6935.43	601.30
IDTRNELESYAYSLKNQIGDKEK	P11021	4	7094.46	679.35
IEIESFYEGEDFSETLTR	P11021	2	10138.13	1083.00
IEWLESHQDADIEDFK	P11021	3	7545.04	658.97
IINEPTAAAIAYGLDK	P11021	2	8020.47	830.45
IINEPTAAAIAYGLDKR	P11021	3	6870.54	606.00
IINEPTAAAIAYGLDKR	P11021	2	6867.05	908.50
ITITNDQNR	P11021	2	2138.96	537.78
ITITNDQNRLTPEEIER	P11021	3	5248.06	681.35
ITPSYVAFTPEGER	P11021	2	6421.94	783.89
ITPSYVAFTPEGERLIGDAAK	P11021	3	7958.74	745.73
KELEEIVQPIISK	P11021	3	6304.49	509.30
KELEEIVQPIISK	P11021	2	6305.72	763.45

KKELEEIVQPIISK	P11021	3	5133.47	552.00
KSDIDEIVLVGGSTR	P11021	3	6037.10	530.29
KSQIFSTASDNQPTVTIK	P11021	3	4607.32	655.68
KSQIFSTASDNQPTVTIK	P11021	2	4611.97	983.02
KTKPYIQVDIGGGQTK	P11021	3	2961.09	578.32
KTKPYIQVDIGGGQTK	P11021	2	2951.68	866.98
KVTHAVVTVPAYFNDAQR	P11021	4	4617.77	504.77
KVTHAVVTVPAYFNDAQR	P11021	3	4612.83	672.69
LIGDAAKNQLTSNPENTVFDAK	P11021	3	6558.55	782.74
LTPEEIER	P11021	2	3254.01	493.76
LYGSAGPPPTGEEDTAEKDEL	P11021	2	5768.97	1088.50
MKETAEAYLGK	P11021	2	2781.25	620.82
M(Oxidation)KETAEAYLGK	P11021	2	2236.90	628.81
MKETAEAYLGKK	P11021	3	2110.37	456.91
M(Oxidation)KETAEAYLGKK	P11021	2	1793.09	692.86
M(Oxidation)KETAEAYLGKK	P11021	3	1796.96	462.24
MKETAEAYLGKK	P11021	2	2108.19	684.86
MVNDAEKFAEEDK	P11021	3	3309.46	509.23
M(Oxidation)VNDAEKFAEEDKK	P11021	3	2051.82	557.26
M(Oxidation)VNDAEKFAEEDKK	P11021	2	2046.91	835.39
MVNDAEKFAEEDKK	P11021	3	2423.62	551.93
M(Oxidation)VNDAEKFAEEDKK...	P11021	3	2498.13	637.66
M(Oxidation)VNDAEKFAEEDKK...	P11021	4	2396.85	549.78
NELESYAYSLK	P11021	2	6436.32	658.82
NQLTSNPENTVFDAK	P11021	2	5446.82	839.41
NQLTSNPENTVFDAKR	P11021	3	4260.53	611.97
NQLTSNPENTVFDAKR	P11021	2	4256.22	917.46
QATKDAGTIAGLNVM(Oxidation...	P11021	3	3539.53	554.63
QATKDAGTIAGLNVM(Oxidation...	P11021	2	3539.12	831.44
RALSSQHQAR	P11021	2	1103.17	577.32
RALSSQHQAR	P11021	3	1103.54	385.21
SDIDEIVLVGGSTR	P11021	2	7895.83	730.88
SQIFSTASDNQPTVTIK	P11021	2	6081.44	918.97
TFAPEEISAMVLTK	P11021	2	9476.05	768.90
TFAPEEISAM(Oxidation)VLTK	P11021	2	7953.70	776.90
TFAPEEISAM(Oxidation)VLTK	P11021	2	9484.35	776.90
TKPYIQVDIGGGQTK	P11021	3	4136.75	535.63
TKPYIQVDIGGGQTK	P11021	2	4133.47	802.94
TWNDPSVQQDIK	P11021	2	4695.89	715.85
VEIIANDQGNR	P11021	2	2876.84	614.82
VLEDSDLKK	P11021	2	1841.47	523.79
VLEDSDLKKSDIDEIVLVGGSTR	P11021	4	7426.59	622.83
VLEDSDLKKSDIDEIVLVGGSTR	P11021	3	7427.12	830.11
VM(Oxidation)EHFIK	P11021	2	1954.59	460.24
VTHAVVTVPAYFNDAQR	P11021	3	5758.44	629.99
VTHAVVTVPAYFNDAQR	P11021	2	5757.18	944.49
VYEGERPLTK	P11021	2	1926.05	596.32
VYEGERPLTK	P11021	3	1926.28	397.88
VYEGERPLTKDNHLLGTFDLTGIPP...	P11021	4	7715.33	777.41

Table 7: Proteins of interest.