

## 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.

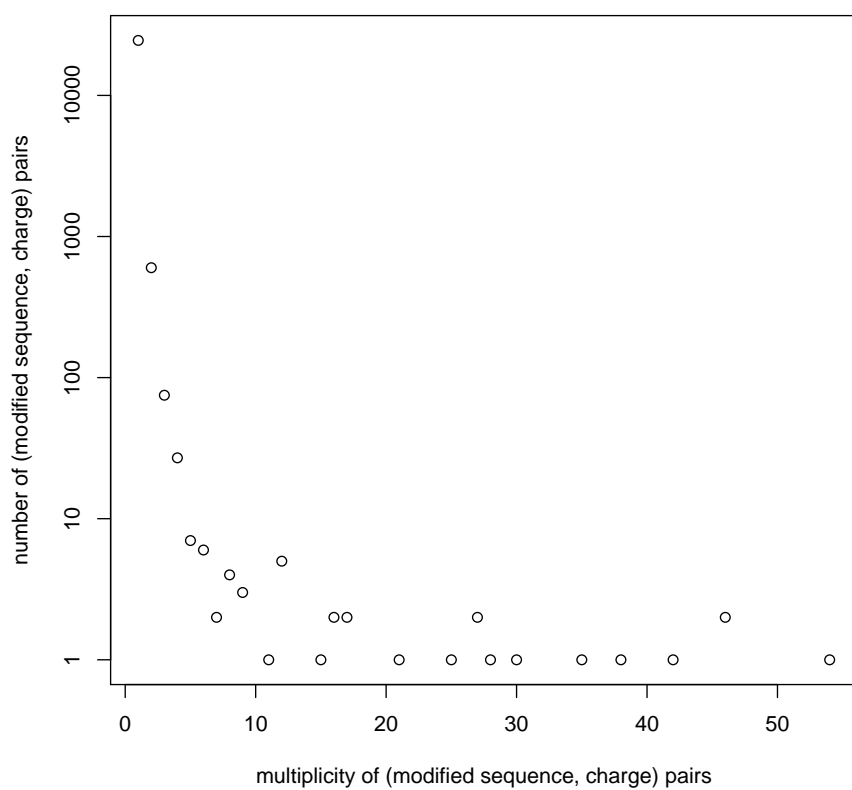
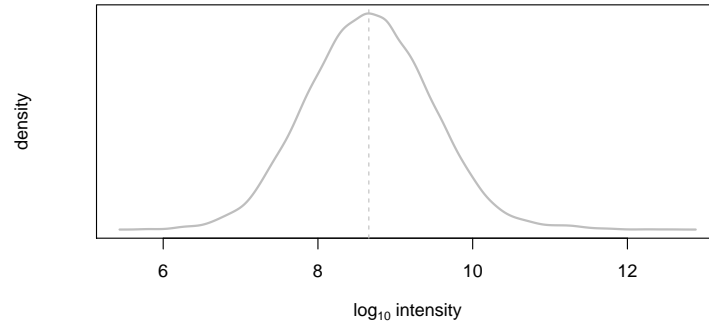
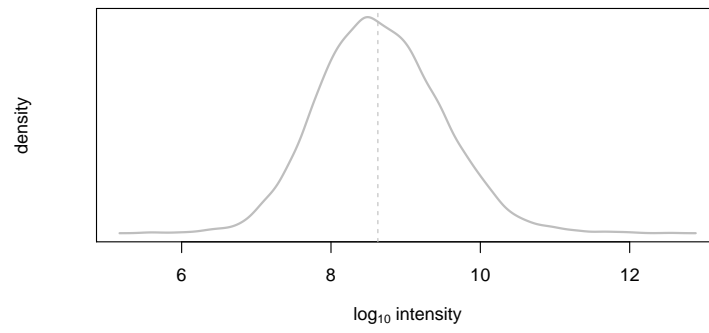


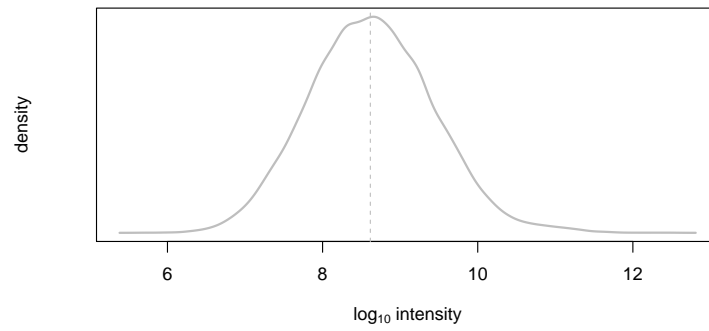
Figure 2: (modified sequence, charge) pair multiplicity vs frequency plot. Each peptide feature (characterised by a (possibly) modified peptide sequence and a charge state) should ideally occur only once in the analysis. In other words, peptides of multiplicity 1 should have a very high frequency. The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

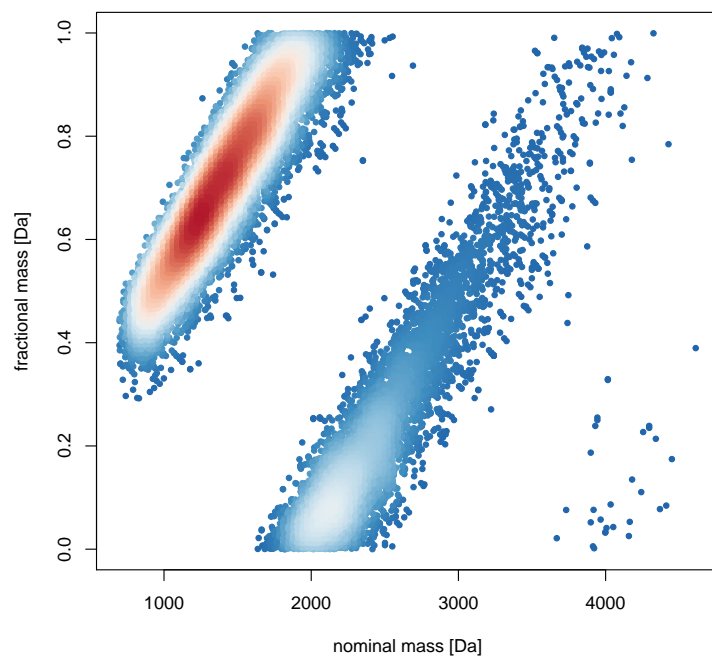


Figure 4: Kendrick nominal fractional mass plot

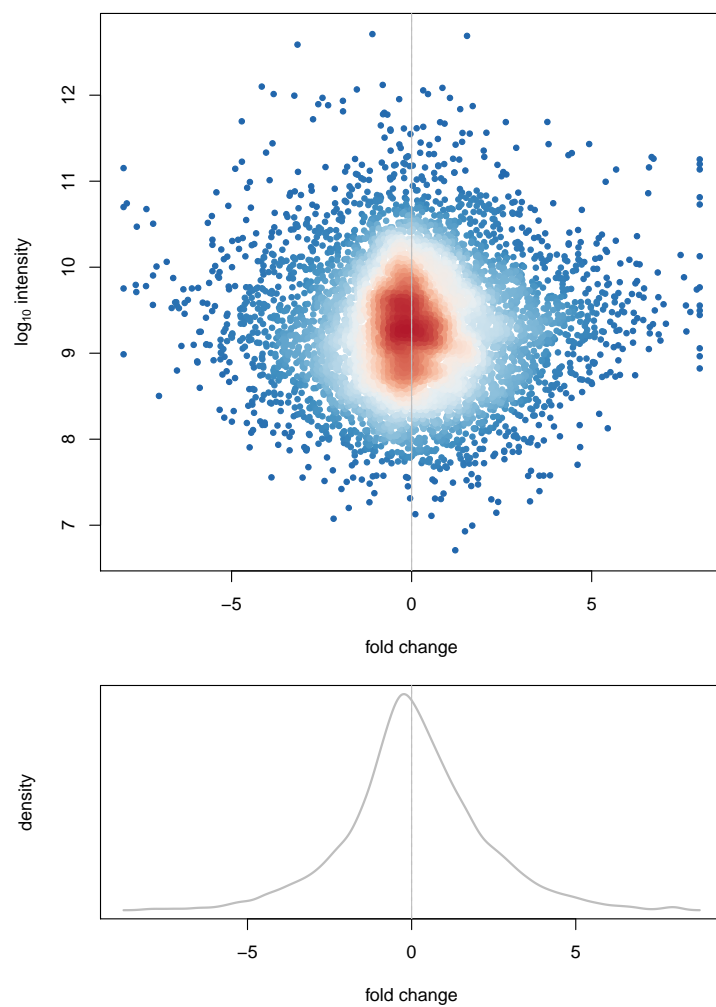


Figure 5: Fold changes of peptide abundances 1 and 2.  
 $\text{median}(\text{fc}) = -0.0026$        $\text{sd}(\text{fc}) = 2.0776$

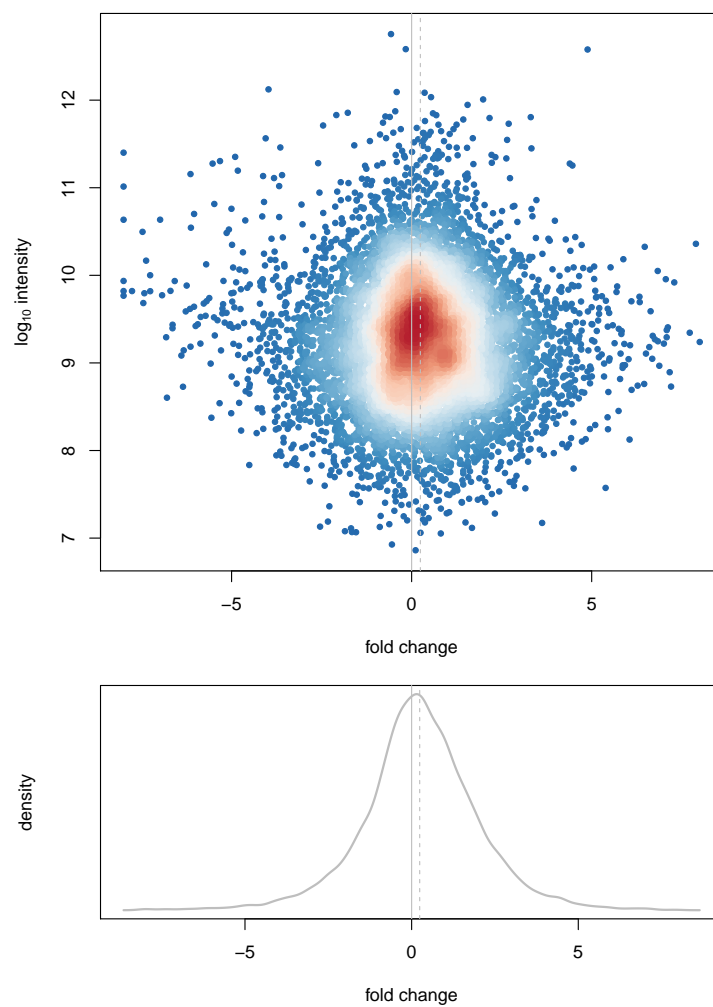


Figure 6: Fold changes of peptide abundances 1 and 3.  
 $\text{median}(\text{fc}) = 0.2421$        $\text{sd}(\text{fc}) = 1.7661$

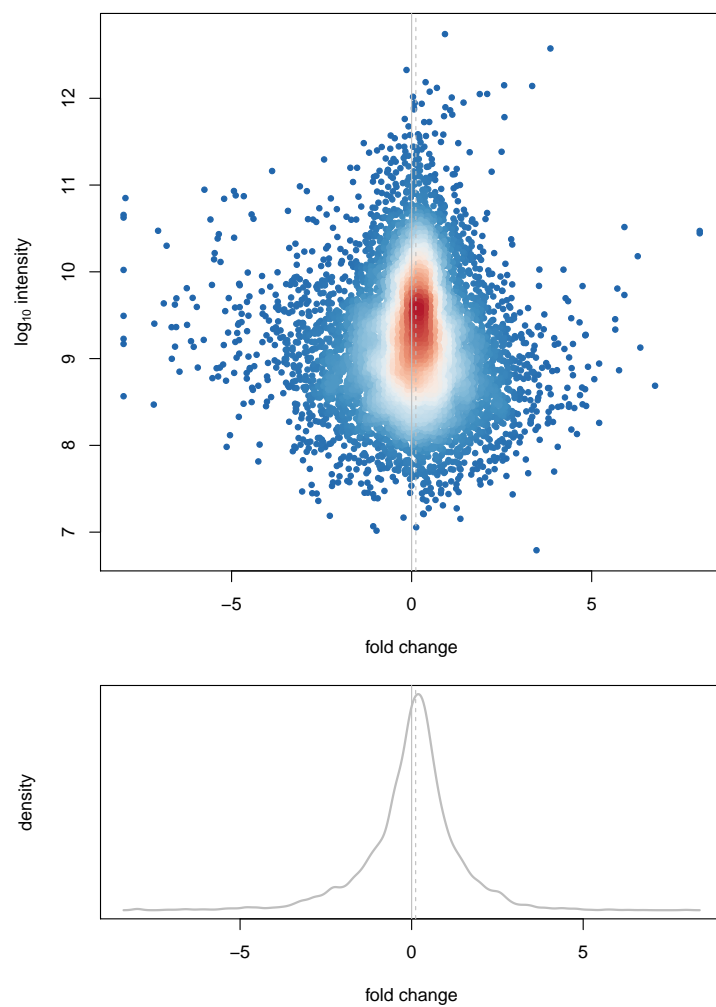


Figure 7: Fold changes of peptide abundances 2 and 3.  
 $\text{median}(\text{fc}) = 0.1175$        $\text{sd}(\text{fc}) = 1.3543$



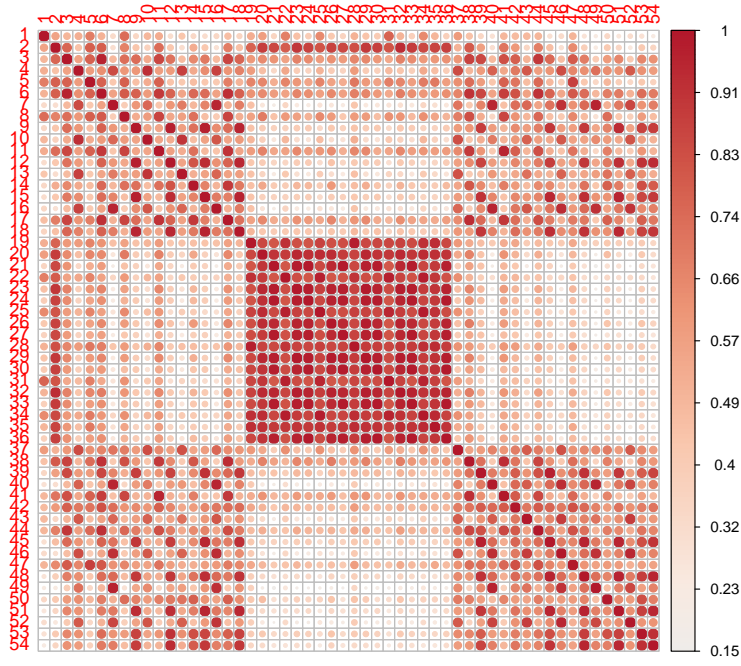


Figure 8: Pearson correlation of all peptide abundances. (min correlation = 0.1484, median correlation = 0.5701, max correlation = 1)

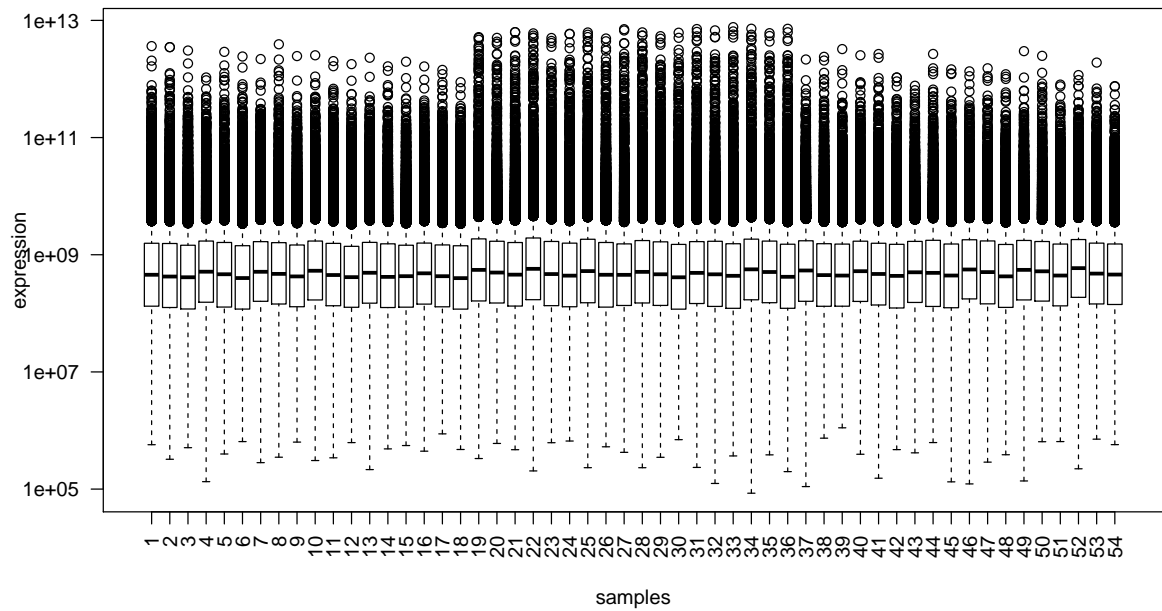


Figure 9: Boxplot of all peptide abundances.

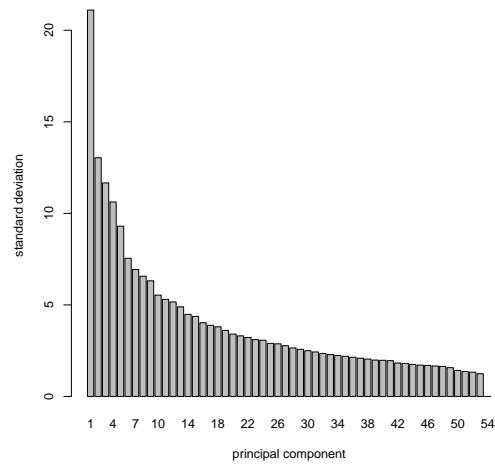


Figure 10: PCA components.

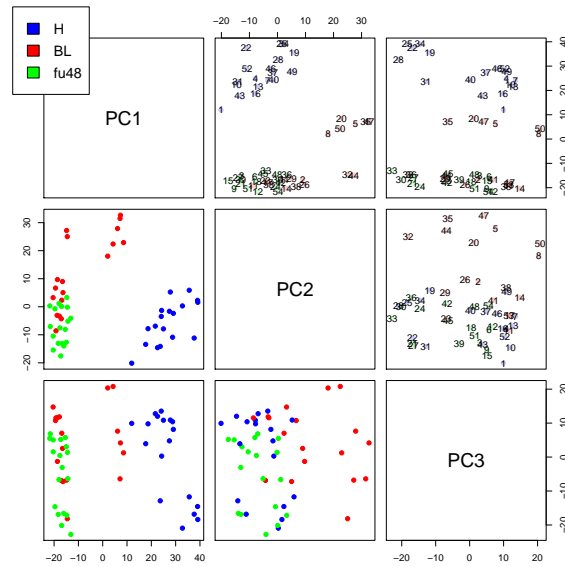


Figure 11: Principal Component Analysis of all peptides with complete quantifications. Any peptides with one or more missing values are ignored.

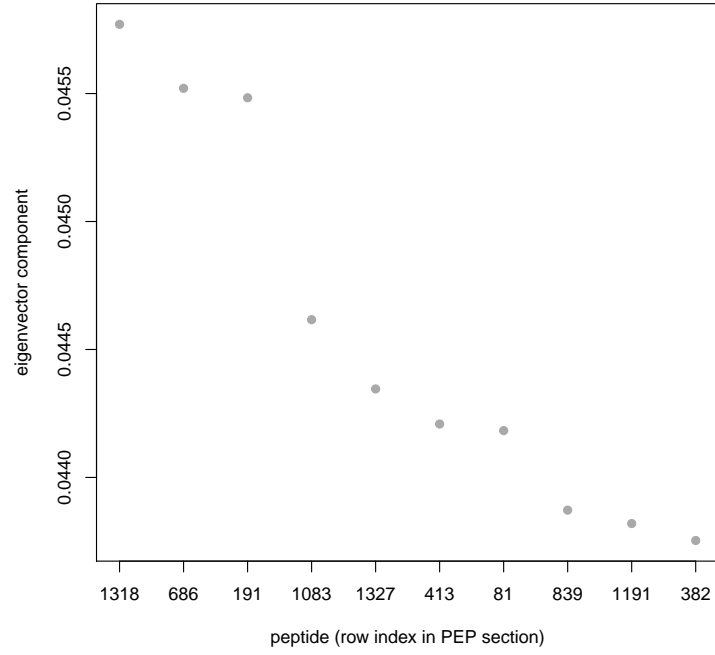


Figure 12: PCA 1st eigenvector.

modified sequence	accession	charge	retention time	m/z
IVAPGKGILAADESTGSIK	P04075	3	5285.58	633.36
YDDM(Oxidation)AAC(Methyl...	P63104	2	2357.93	563.19
VISGVLQLGNIVFKK	P35579	3	8817.89	539.00
NKPLEQSVEDLSKGPPSSVPK	O95466	3	5083.06	746.07
IANLQTDLSDDLGR	P21333	2	6841.42	708.38
LIDFLEC(Methylthio)GK	P17844	2	9345.30	542.26
SAVGFNEM(Oxidation)EAPTTA...	P14317	3	3498.83	620.63
TIIPILISQC(Methylthio)TPK	P40926	2	9466.64	680.37
RTGAIVDVPVGEELLGR	P25705	3	7675.89	594.34
SETAPAAPAAPAPAEKTPVKK	P10412	3	2224.46	678.04

Table 3: PCA 1st eigenvector.

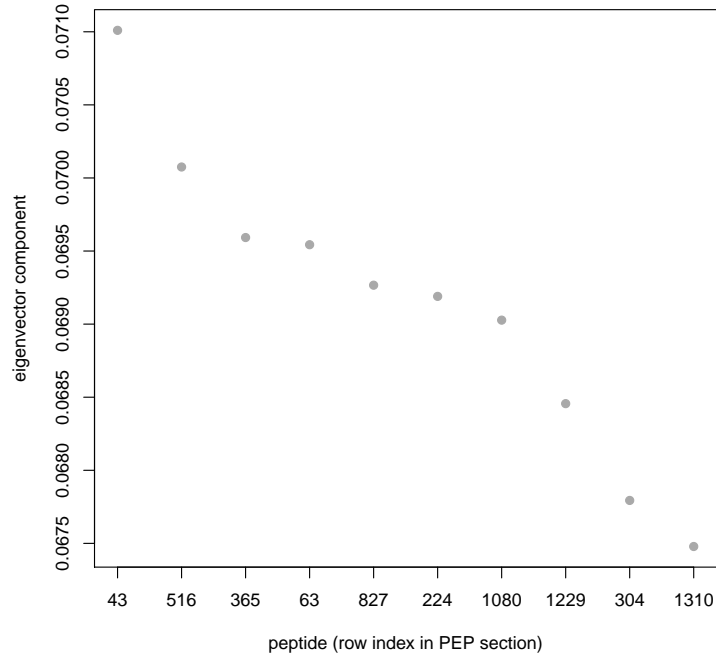


Figure 13: PCA 2nd eigenvector.

modified sequence	accession	charge	retention time	m/z
STPEYFAER	P08133	2	3515.19	550.26
KQPPVSPGTALVGSQKEPSEVPTPK	P17096	3	4226.12	853.47
DNHLLGTFDLTGIPPAPR	P11021	3	9496.78	645.34
DREVGIPPEQSLETAK	P61158	3	4602.34	590.31
GLPDPALSTQPAPASR	Q14005	2	5190.93	789.42
LQFHDVAGDIFHQQC(Methylthi...	P11413	4	7201.68	483.73
VNLSAAQTLR	Q9BUL8	2	4025.03	536.81
ISGASEKDIVHSGLAYTM(Oxidat...	P00367	4	5040.61	545.77
HVLTSIGEK(Label:13C(6)15N...	STD_03	2	2127.71	496.29
HGGTIPIVPTAEFQDR	P00367	3	6115.00	579.97

Table 4: PCA 2nd eigenvector.

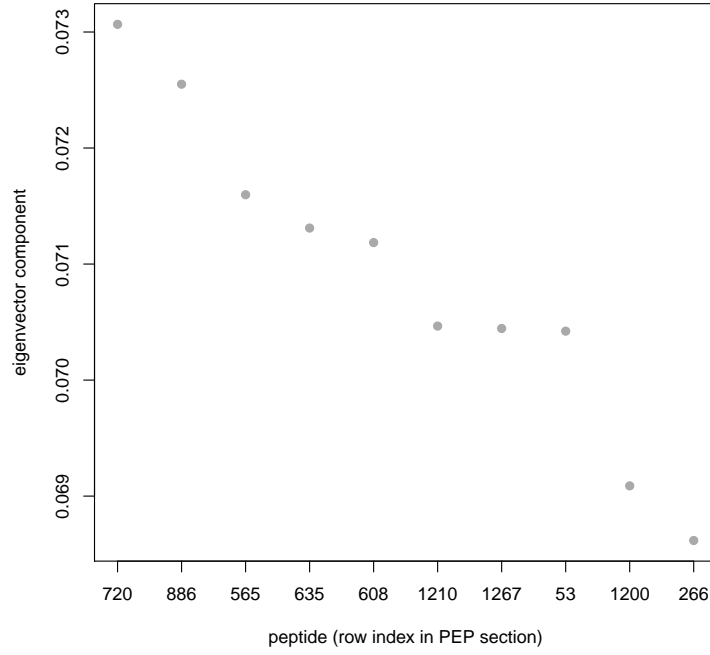


Figure 14: PCA 3rd eigenvector.

modified sequence	accession	charge	retention time	m/z
IAFAITAIK	P62269	2	7044.51	474.30
GITGVEDKESWHGKPLPK	P29401	3	2940.99	660.02
VALVYGMNEPPGAR	P06576	2	5752.97	801.40
SSANVEEAFFTLAR	Q92930	2	9328.50	771.38
SM(Oxidation)YEEEINETR	P20700	2	3224.81	708.80
FLIDGFPR	P30085	2	8094.48	482.77
AGVAPLQVK	P21333	2	3134.86	441.77
TETQEKNPLPSKETIEQEK	P62328	3	2708.84	743.71
VM(Oxidation)VQPINLIFR	P62304	2	9095.18	673.39
AVEVQGSPSLESGDHGK	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
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
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
AIMTYVSSFYHAFSQAQK	O43707	3	9592.08	669.99
AIMTYVSSFYHAFSQAQK	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
AIMTYVSSFYHAFSQAQKAETAANR	O43707	3	8754.95	907.77
ALDFIASK	O43707	2	4963.37	432.74
ASFNHFDKDHGGALGPPEEFK	O43707	4	4122.09	551.51
ASFNHFDKDHGGALGPPEEFK	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
ETTDTDADQVIASFK	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
IAESNHK	O43707	2	1235.63	456.25
IAESNHKLSGSNPYTTVTPQIINS...	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
LMLLEVISGERLPKPER	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
LSNRPAFMPSEK	O43707	3	3100.77	478.58
LVSIGAEIIVDGNK	O43707	2	6663.17	757.91
M(Oxidation)APYQGPDVPGAL...	O43707	2	6433.07	904.93
MAPYQGPDVPGALDYK	O43707	2	7001.32	896.93
M(Oxidation)APYQGPDVPGAL...	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
QFASQANVVGPWQITK	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
RQFASQANVVGVPWIQTK	O43707	3	5919.51	644.01
RTIPWLEDRVPQK	O43707	3	4602.85	546.64
SIVDYKPNLDLLEQQHQHQLIQEALIF...	O43707	4	11309.39	831.94
SIVDYKPNLDLLEQQHQHQLIQEALIF...	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
VGWEQLTTIAR	O43707	2	11063.02	693.89
VHKPPKVQEK	O43707	3	1081.02	397.24
VHKPPKVQEK	O43707	2	1104.93	595.36
VLADGKNFITAEELR	O43707	3	5870.35	559.31
VLADGKNFITAEELR	O43707	2	5867.80	838.45
VLADGKNFITAEELRR	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
RALSSQHQR	P11021	2	1103.17	577.32
RALSSQHQR	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
VEIHANDQGNR	P11021	2	2876.84	614.82
VLEDSLKK	P11021	2	1841.47	523.79
VLEDSLKKSDIDEIVLVGGSTR	P11021	4	7426.59	622.83
VLEDSLKKSDIDEIVLVGGSTR	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.