

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

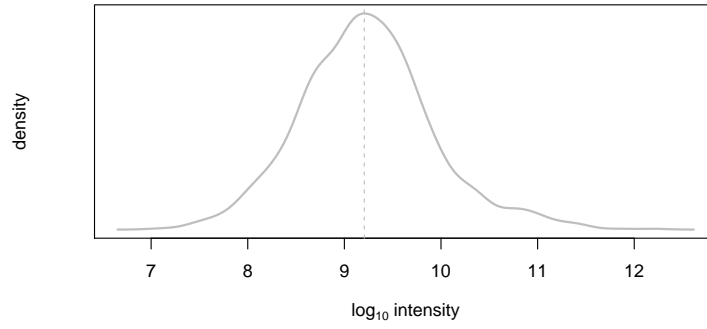
Table 2: Statistics of modifications.



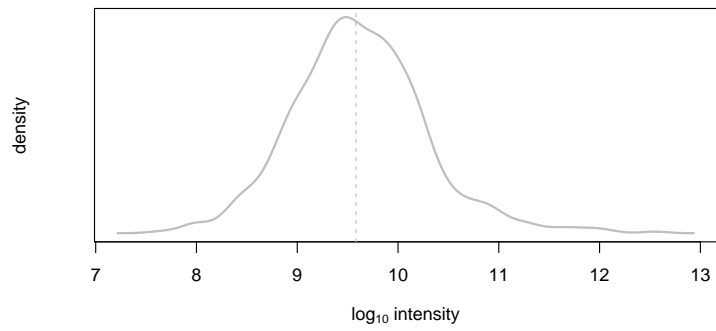
Figure 1: Frequency plot of peptide quantifications.



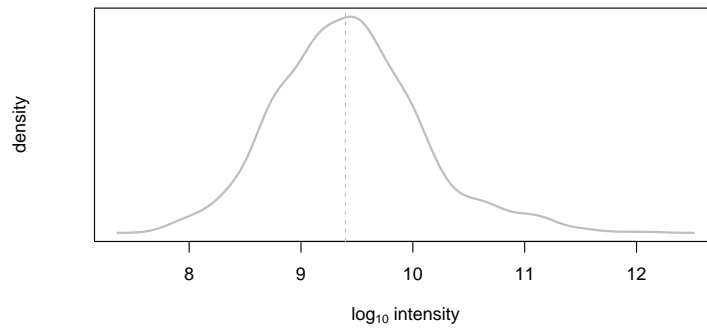
Figure 2: (modified sequence, charge) pair multiplicity vs frequency plot. Each peptide feature (characterised by a (possibly) modified peptide sequence and a charge state) should ideally occur only once in the analysis. In other words, peptides of multiplicity 1 should have a very high frequency. The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

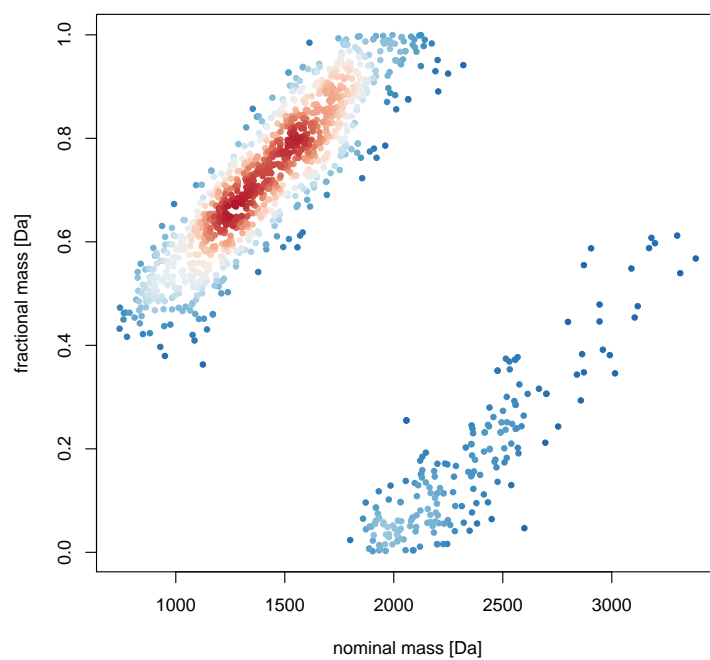


Figure 4: Kendrick nominal fractional mass plot

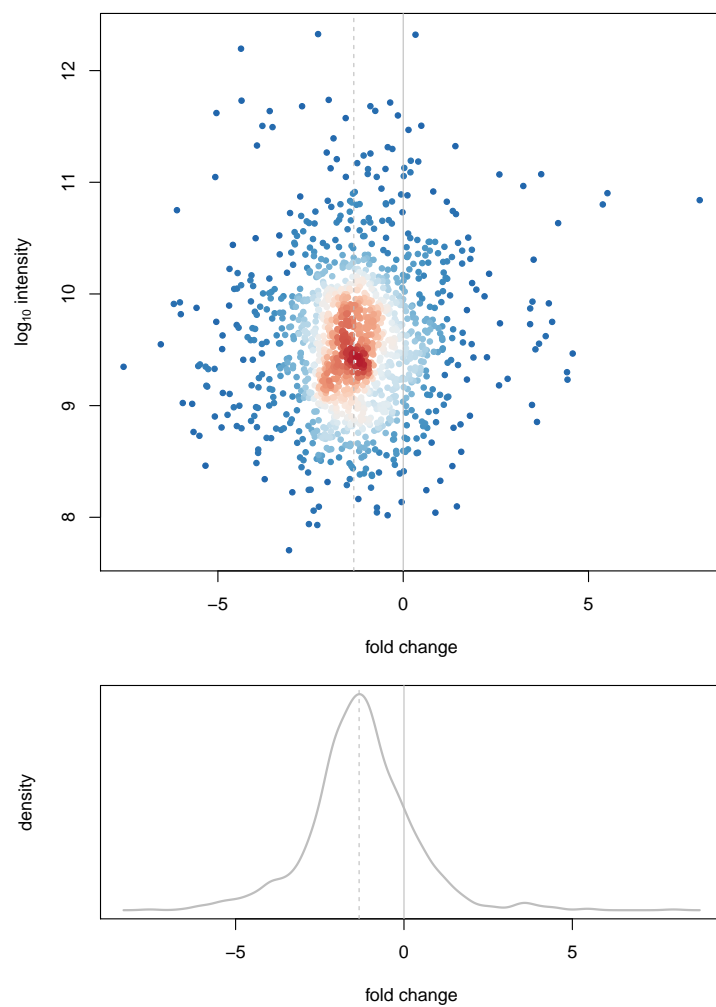


Figure 5: Fold changes of peptide abundances 1 and 2.
 $\text{median}(\text{fc}) = -1.3328$ $\text{sd}(\text{fc}) = 1.5445$

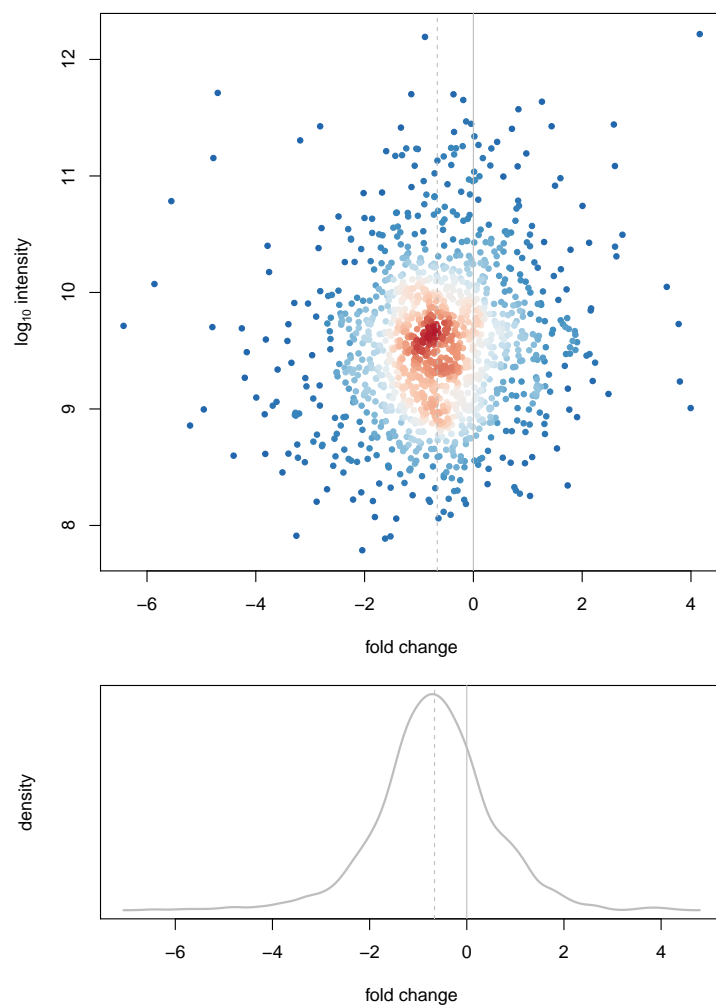


Figure 6: Fold changes of peptide abundances 1 and 3.
 $\text{median}(\text{fc}) = -0.6641$ $\text{sd}(\text{fc}) = 1.1804$

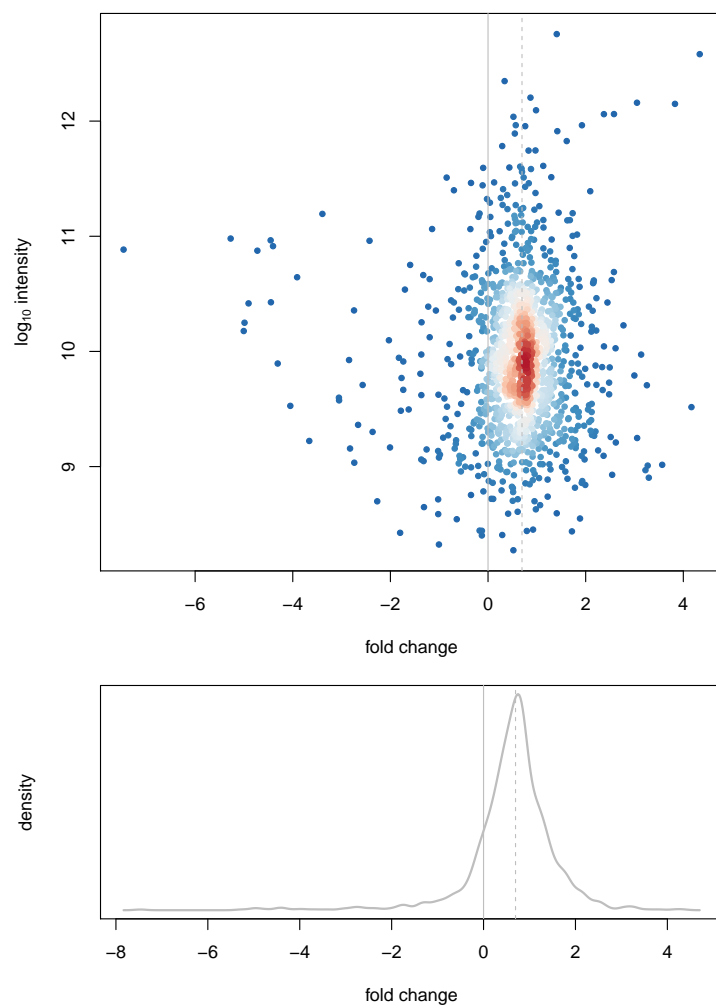


Figure 7: Fold changes of peptide abundances 2 and 3.
 $\text{median}(\text{fc}) = 0.6958$ $\text{sd}(\text{fc}) = 0.9636$

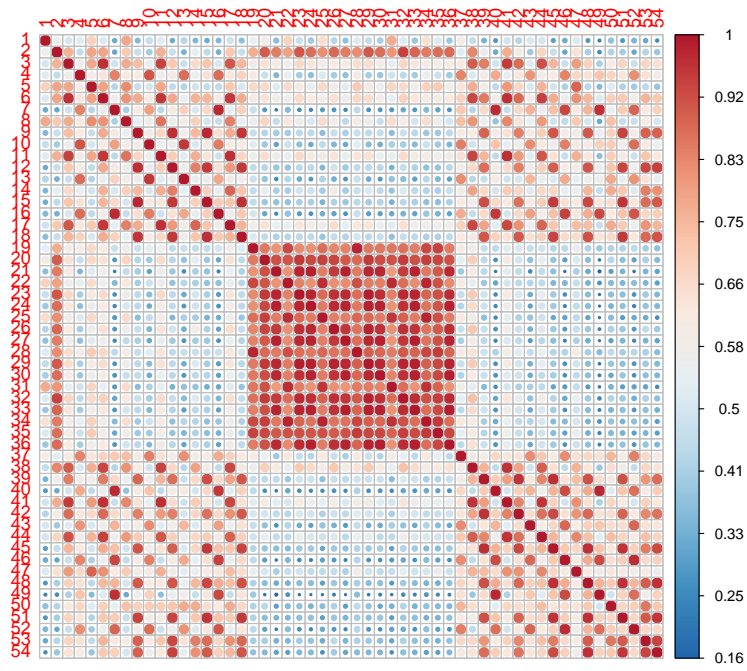


Figure 8: Pearson correlation of all peptide abundances. (min correlation = 0.1622, median correlation = 0.5936, max correlation = 1)

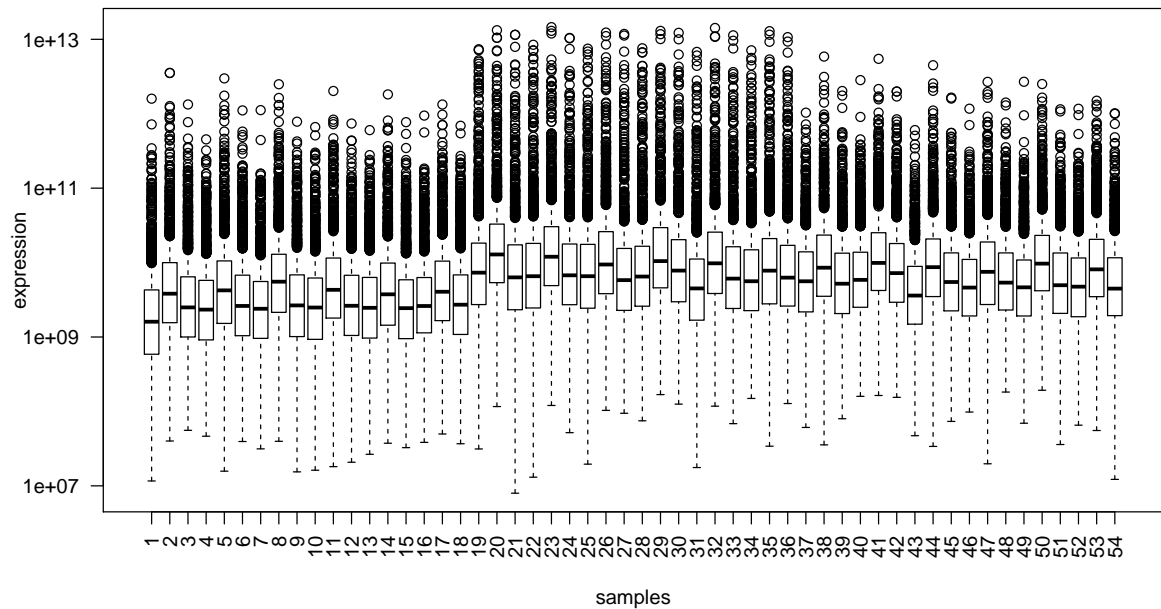


Figure 9: Boxplot of all peptide abundances.

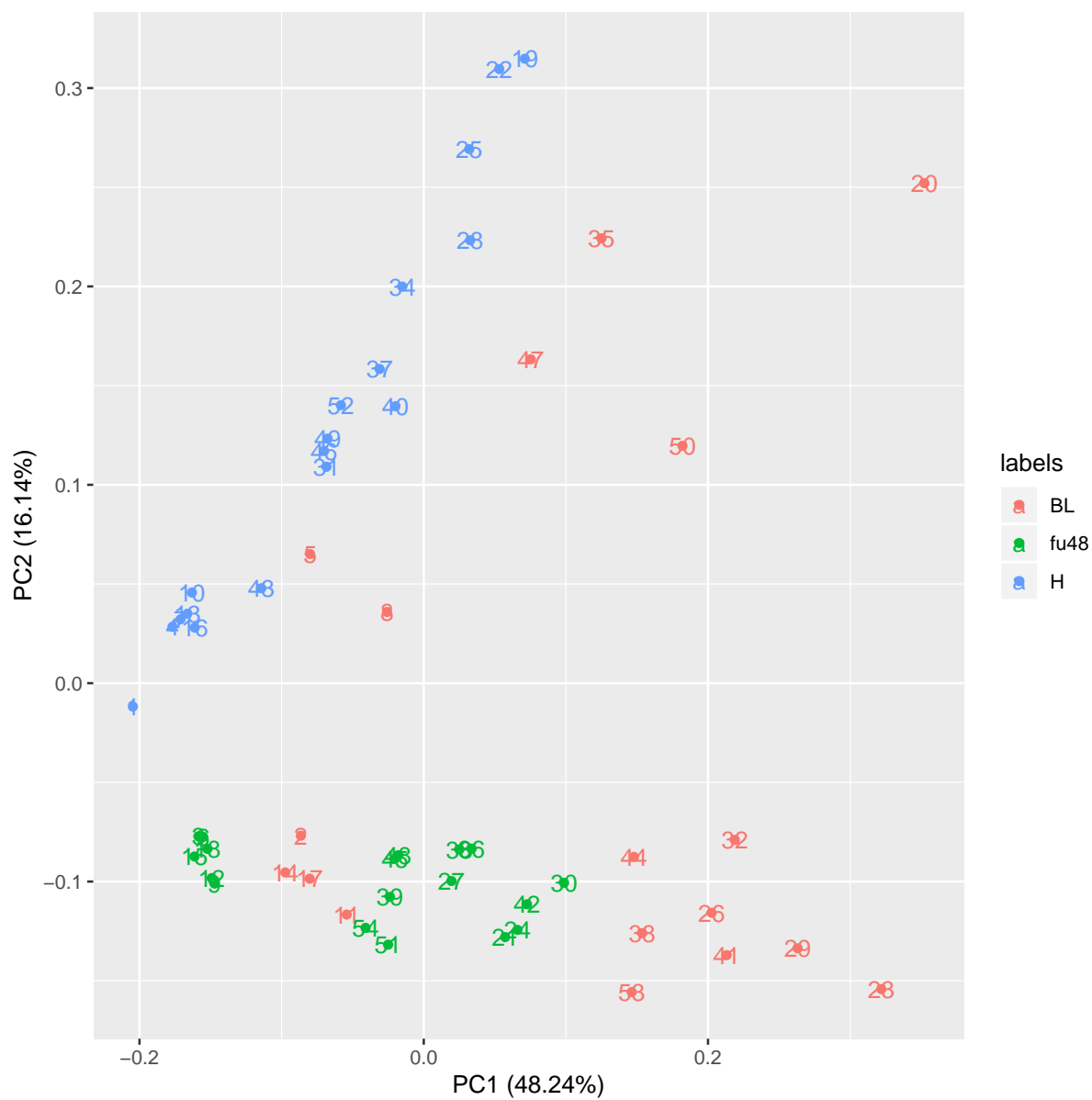


Figure 10: Principal Component Analysis of all peptides with complete quantifications. Any peptides with one or more missing values are ignored.

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

Table 3: 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
AHGGYSVFAGVGER	P06576	3	4066.84	469.57
FLSQPFQVAEVFTGHM(Oxidatio...	P06576	3	8779.41	680.34
FTQAGSEVSALLGR	P06576	2	7458.45	718.38
IM(Oxidation)DPNIVGSEHYDV...	P06576	3	4749.42	611.29
IM(Oxidation)NVIGEPIDERGP...	P06576	3	5343.69	599.66
LVLEVAQHLGESTVR	P06576	3	6607.33	550.98
TIAM(Oxidation)DGTEGLVR	P06576	2	4113.14	639.82
VALVYGQM(Oxidation)NEPPGA...	P06576	2	4560.45	809.41
VLDSGAPIKIPVGPETLGR	P06576	3	7703.51	640.37
VLDSGAPIKIPVGPETLGR	P06576	2	7703.86	960.05
VVDLLAPYAK	P06576	2	7025.47	544.82
GFAFVQYVNER	P07910	2	7451.91	665.33
M(Oxidation)IAGQVLDINLAAE...	P07910	2	8127.15	849.96
MIAGQVLDINLAAEPK	P07910	2	8833.20	841.96
VPPPPPIAR	P07910	2	3073.40	472.29
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
ETTDTDADQVIASFK	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
VYGERPLTK	P11021	2	1926.05	596.32
IYVDDGLISLQVK	P14618	2	8923.18	731.91
KGVNLPAAVDLPAVSEKDIQDLK	P14618	4	7868.62	620.10
KGVNLPAAVDLPAVSEKDIQDLK	P14618	3	7867.84	826.46
SVETLKEM(Oxidation)IK	P14618	2	2674.97	597.33
LIDFLEC(Methylthio)GK	P17844	2	9345.30	542.26
IASLEVENQSLR	P29692	2	5007.93	679.87
SLAGSSGPGASSGTSGDHGELVVR	P29692	3	3552.50	729.02
EATNPPVIQEEKPK	P30101	3	2402.50	527.28

FLQDYFDGNLKR	P30101	3	6540.39	505.92
FVM(Oxidation)QEEFSR	P30101	2	3414.10	594.77
GFPTIYFSPANK	P30101	2	7787.46	671.35
GFPTIYFSPANKK	P30101	2	5901.08	735.39
GFPTIYFSPANKK	P30101	3	5900.67	490.60
IFRDGEEAGAYDGPR	P30101	2	3383.93	826.89
IFRDGEEAGAYDGPR	P30101	3	3384.40	551.59
LKGIVPLAK	P30101	2	3181.18	469.82
LSKDPNIVIAK	P30101	2	2868.45	599.36
M(Oxidation)DATANDVPSPYEV...	P30101	2	5066.94	840.88
YGVSGYPTLK	P30101	2	4804.40	542.79
AGGIETIANEYSDR	P34932	2	5849.11	748.35
AIADTGANVVVTGCK	P50990	2	4341.17	686.87
HFSGLEEAVYR	P50990	2	4456.90	654.32
LVPGGGATEIELAK	P50990	2	5643.63	677.88
NLRDIDEVSSLLR	P50990	3	7752.87	510.61

Table 4: Proteins of interest.