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.

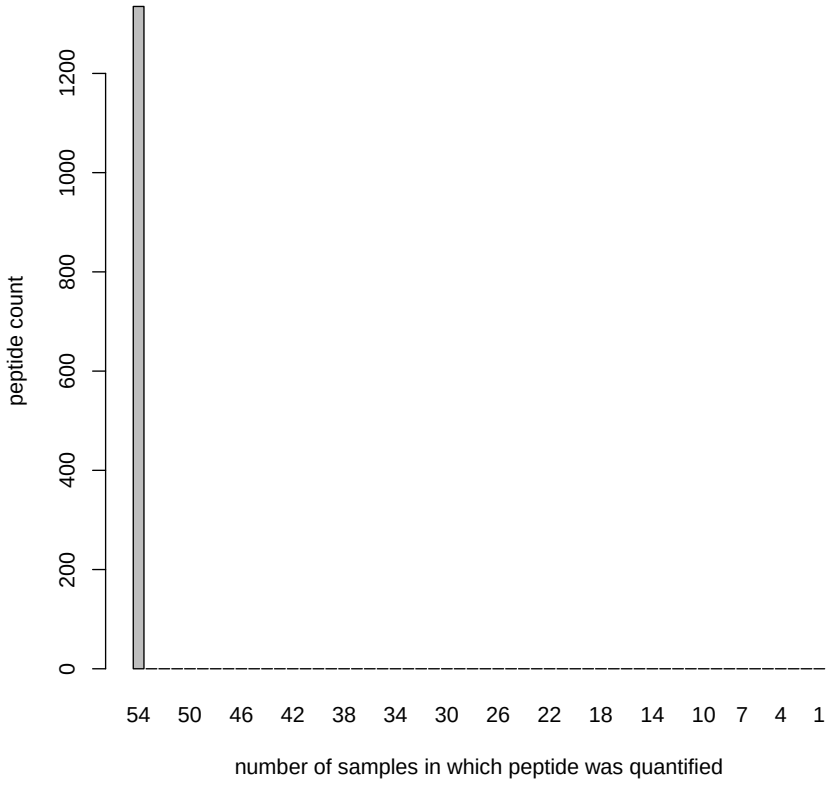


Figure 1: Frequency plot of peptide quantifications.

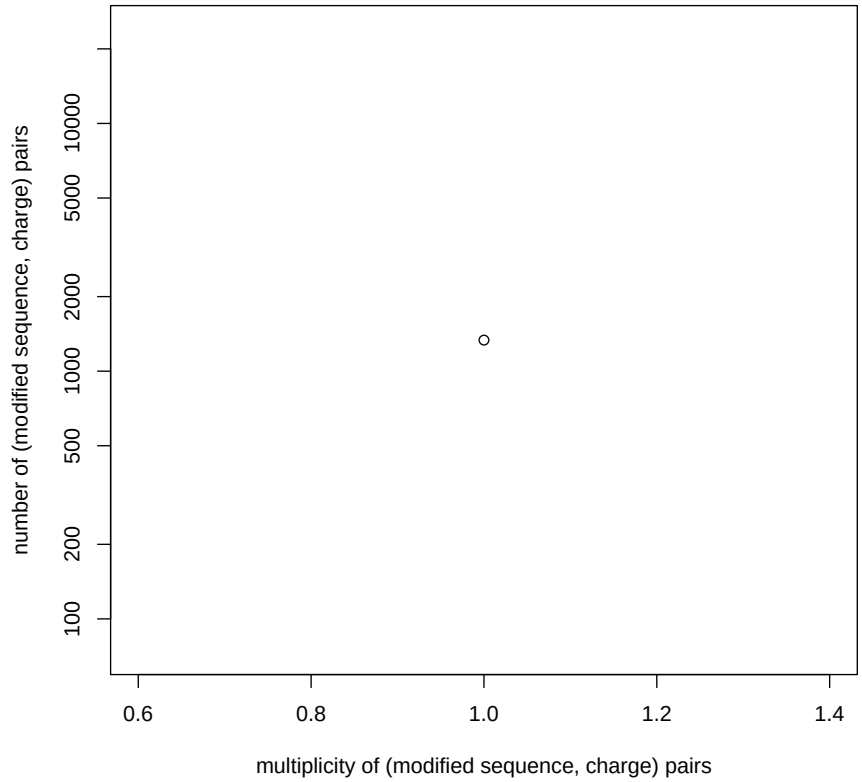
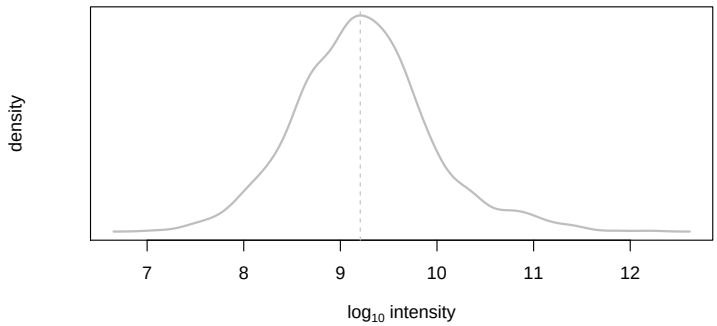
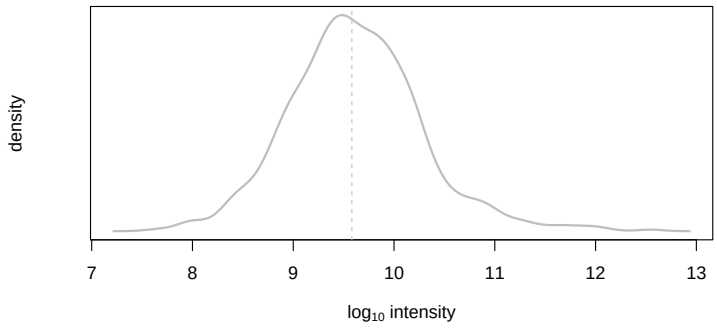


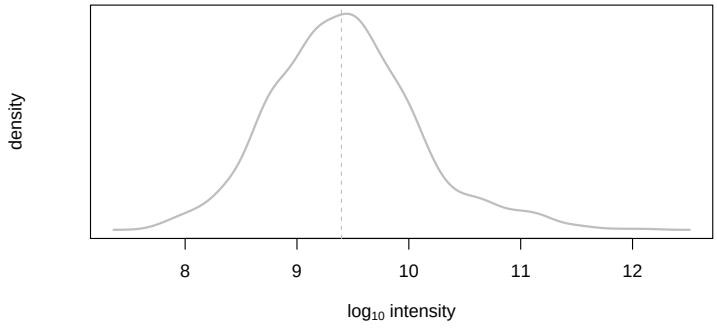
Figure 2: (modified sequence, charge) pair multiplicity vs frequency plot. Each peptide feature (characterised by a (possibly) modified peptide sequence and a charge state) should ideally occur only once in the analysis. In other words, peptides of multiplicity 1 should have a very high frequency. The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

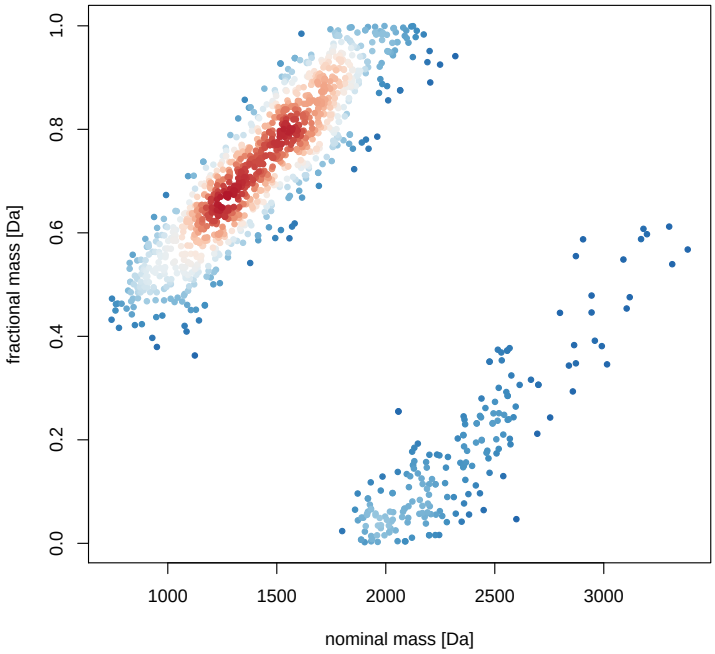


Figure 4: Kendrick nominal fractional mass plot

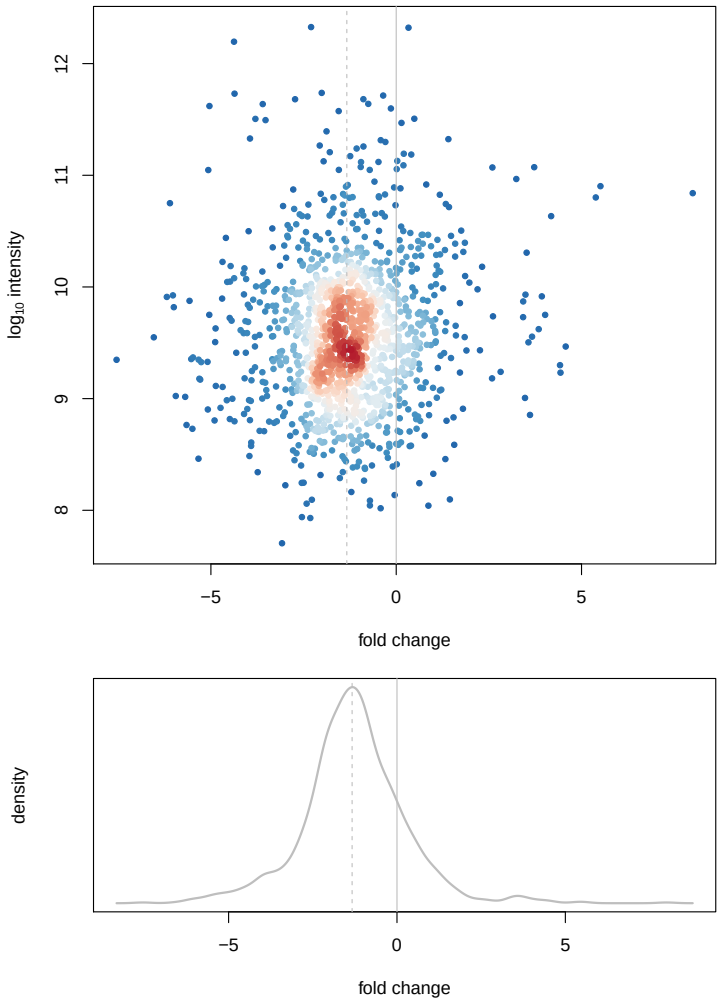


Figure 5: Fold changes of peptide abundances 1 and 2.
median(fc) = −1.3328 sd(fc) = 1.5445

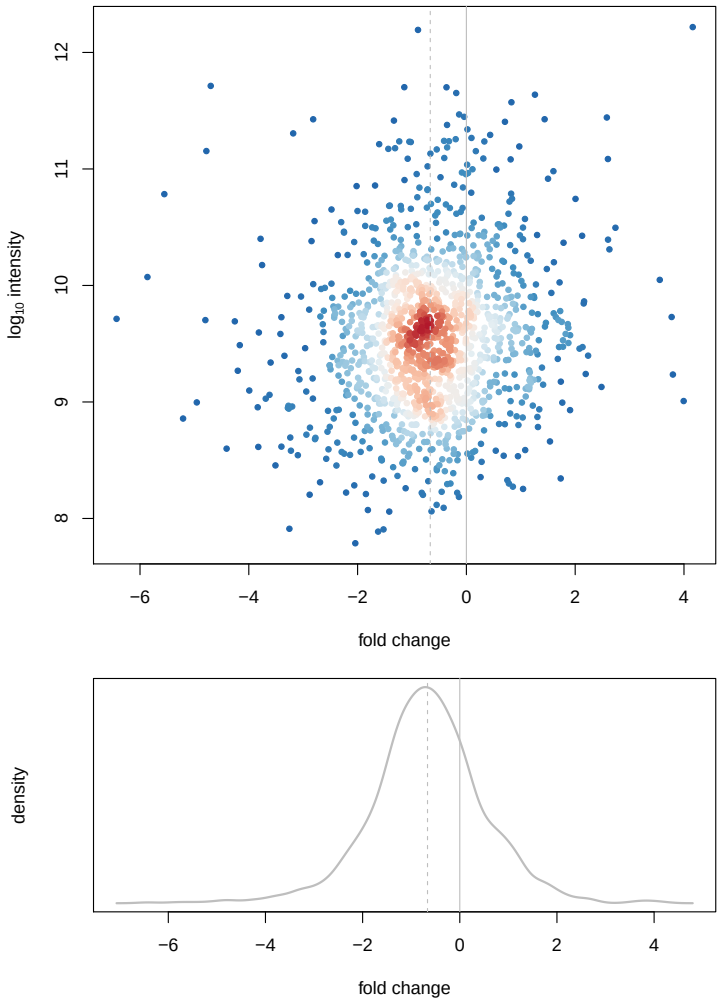


Figure 6: Fold changes of peptide abundances 1 and 3.
median(fc) = −0.6641 sd(fc) = 1.1804

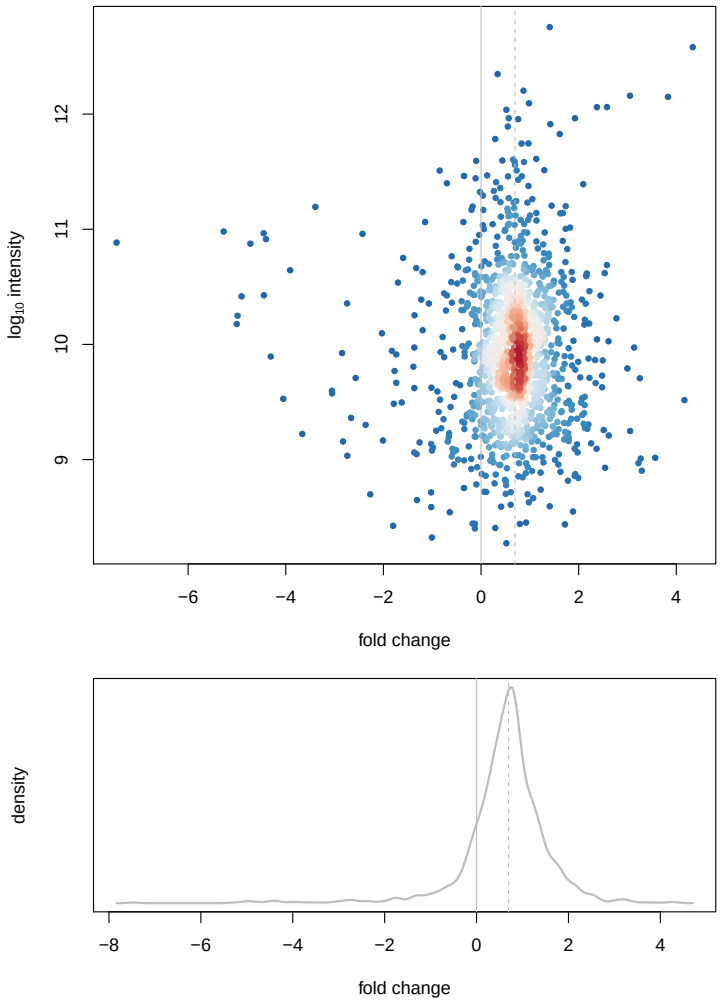


Figure 7: Fold changes of peptide abundances 2 and 3.
median(fc) = 0.6958 sd(fc) = 0.9636

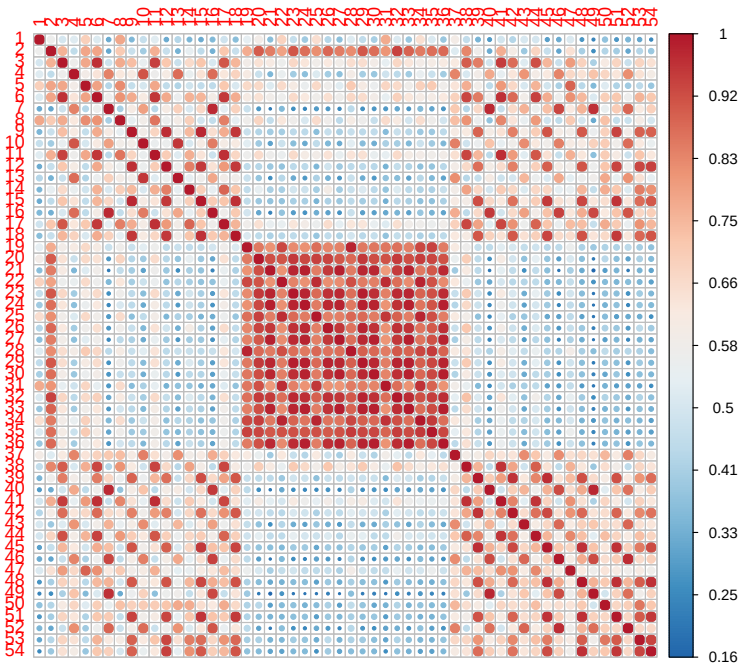


Figure 8: Pearson correlation of all peptide abundances. (min correlation = 0.1622, median correlation = 0.5936, max correlation = 1)

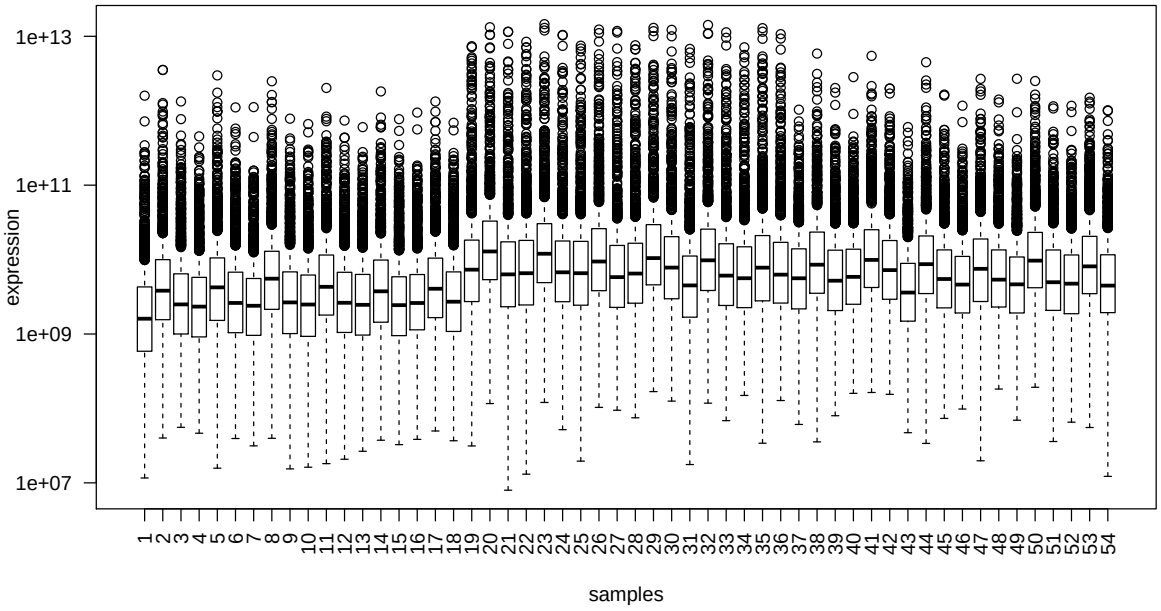


Figure 9: Boxplot of all peptide abundances.

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
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
IYVDDGLISLQVK	P14618	2	8923.18	731.91
KGVNLPGAAVDLPAVSEKDIQDLK	P14618	4	7868.62	620.10
KGVNLPGAAVDLPAVSEKDIQDLK	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
AIADTGANVVVTGGK	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.