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.

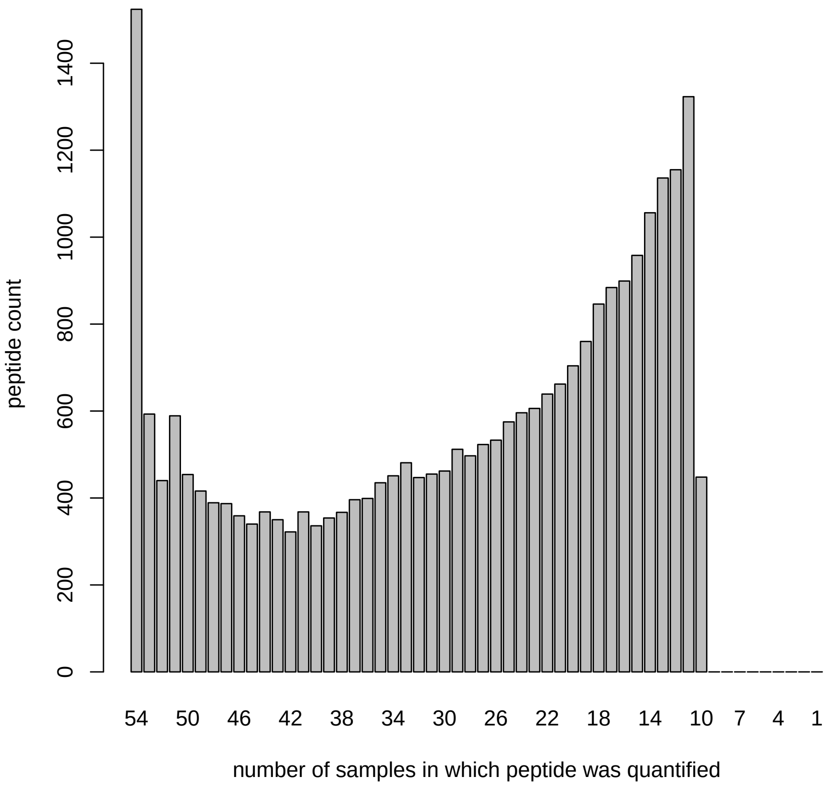


Figure 1: Frequency plot of peptide quantifications.

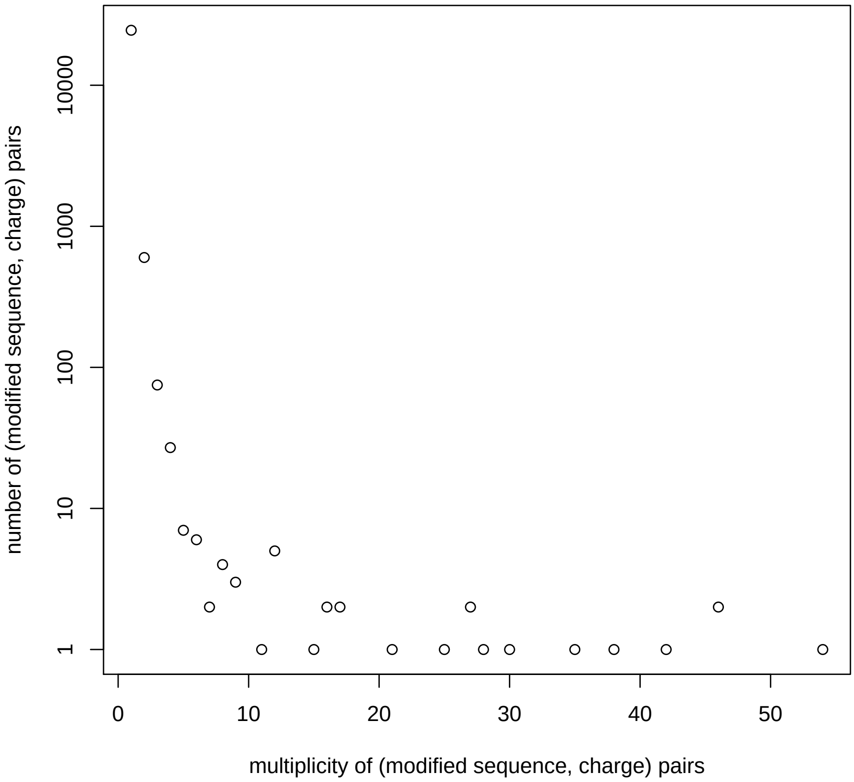
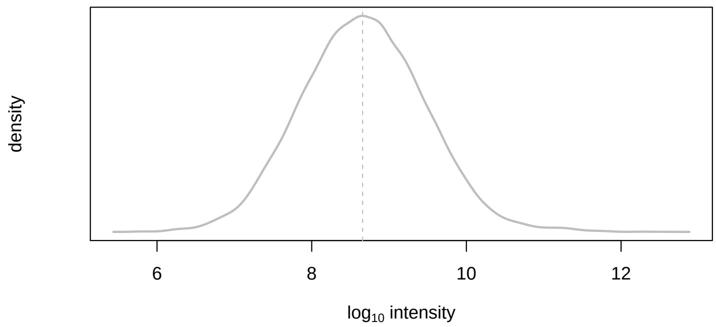
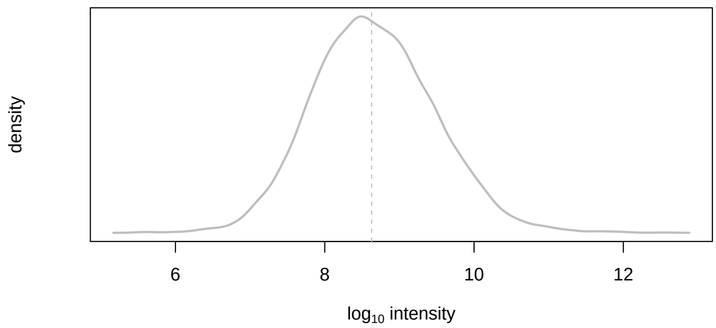


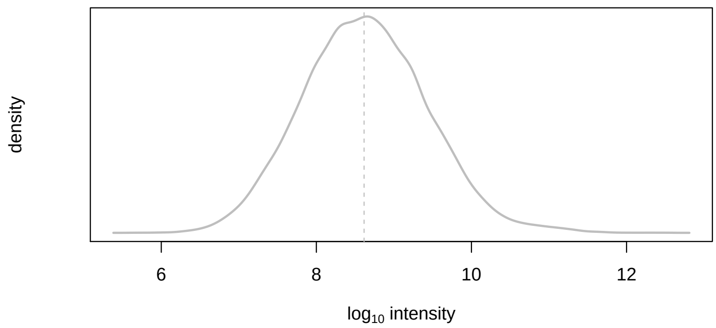
Figure 2: (modified sequence, charge) pair multiplicity vs frequency plot. Each peptide feature (characterised by a (possibly) modified peptide sequence and a charge state) should ideally occur only once in the analysis. In other words, peptides of multiplicity 1 should have a very high frequency. The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

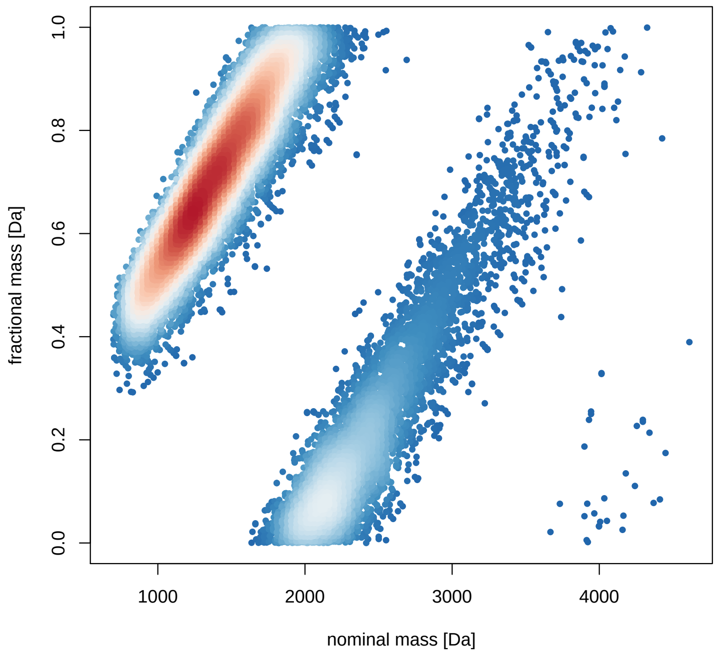


Figure 4: Kendrick nominal fractional mass plot

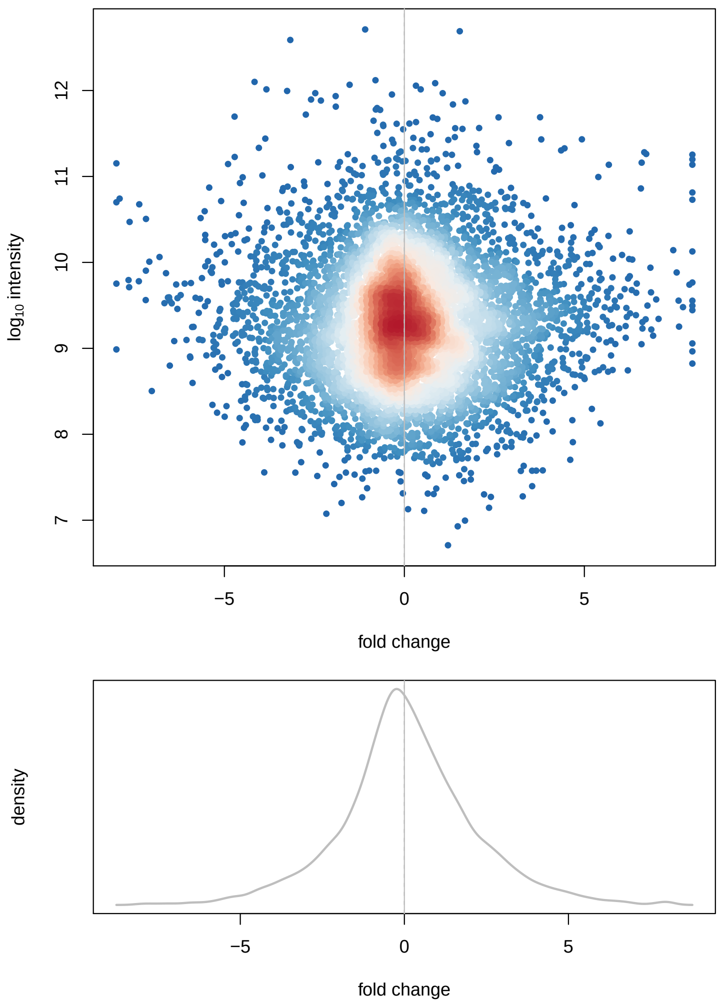


Figure 5: Fold changes of peptide abundances 1 and 2.
median(fc) = −0.0026 sd(fc) = 2.0776

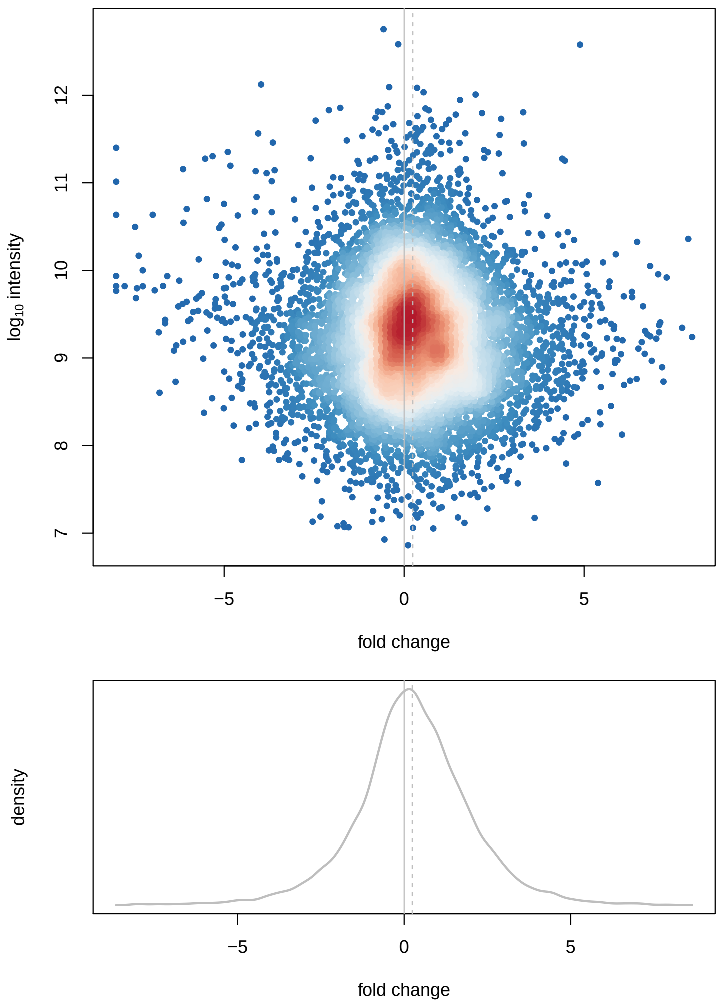


Figure 6: Fold changes of peptide abundances 1 and 3.
median(fc) = 0.2421   sd(fc) = 1.7661

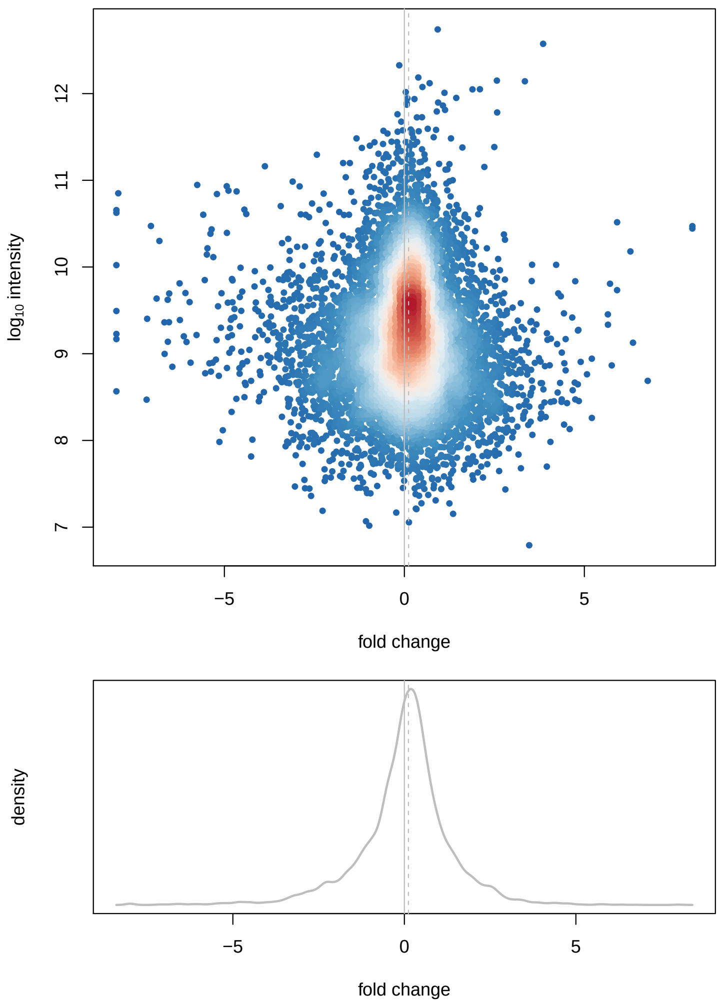


Figure 7: Fold changes of peptide abundances 2 and 3.
median(fc) = 0.1175 sd(fc) = 1.3543

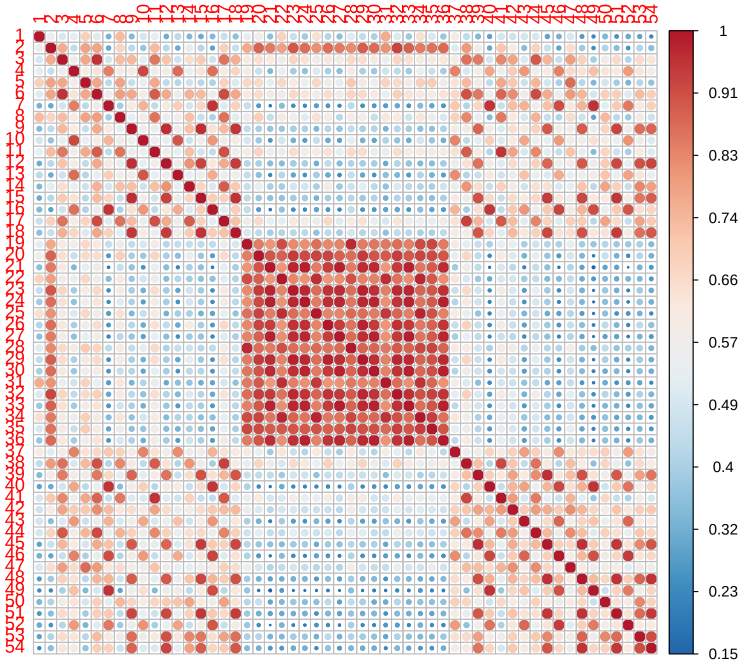


Figure 8: Pearson correlation of all peptide abundances. (min correlation = 0.1484, median correlation = 0.5701, max correlation = 1)

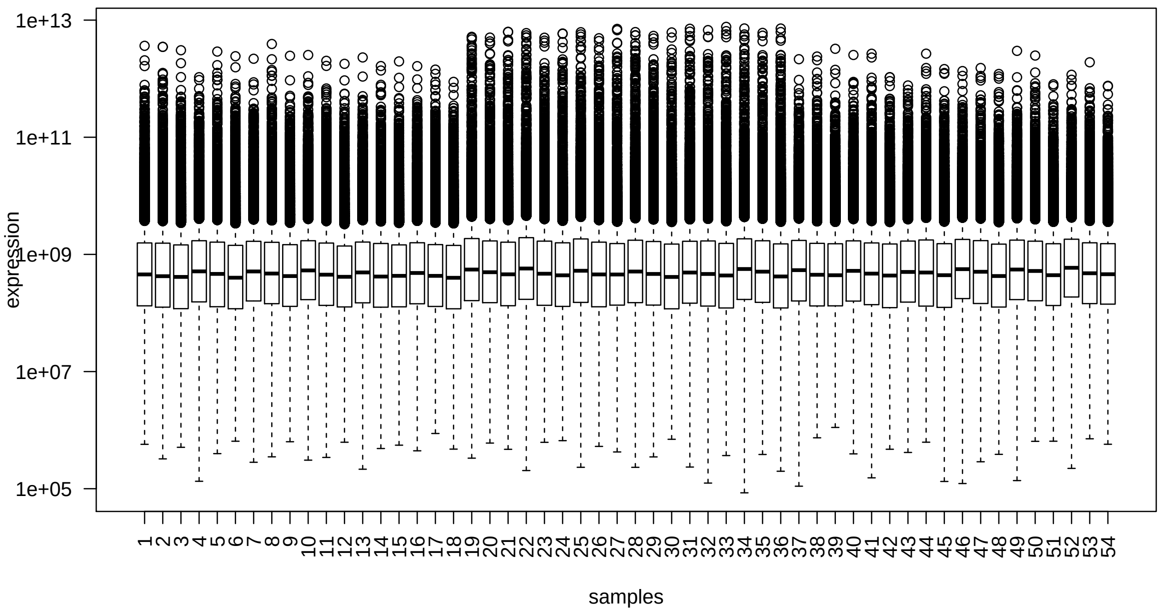


Figure 9: Boxplot of all peptide abundances.

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(Methylthio)YNC(Methylthio)GKPGHLAR	P62633	4	4025.06	454.93
EQC(Methylthio)C(Methylthio)YNC(Methylthio)GKPGHLAR	P62633	3	4045.75	606.23
M(Oxidation)VQEAEKYKAEDEKQR	P11142	4	1316.10	500.25
M(Oxidation)VQEAEKYKAEDEKQR	P11142	3	1320.29	666.66
MVQEAEKYKAEDEKQR	P11142	3	1585.13	661.33
M(Oxidation)VQEAEKYKAEDEKQR	P11142	2	1324.47	999.48
MVQEAEKYKAEDEKQR	P11142	4	1577.81	496.25
TVPFC(Methylthio)STFAAFFTR	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 3: Peptides of interest. 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
AALETDENLLLC(Methylthio)APTGAGK	O75643	2	9446.27	966.97
ANSNLVLQADR	O75643	2	3364.48	600.82
DILC(Methylthio)GAADEVLAVLK	O75643	2	13363.36	788.41
GLFYFDNSFRPVPLEQTYVGITEK	O75643	3	10851.51	940.81
GNIIISTPEKWDILSR	O75643	3	8401.82	614.67
GYTLLSEGIDEMVGIIYKPK	O75643	3	12026.42	742.73
HLILPEKYPPPTELLDLQPLPVSALR	O75643	4	10522.78	738.18
HLSDHLSELVEQTLSDLEQSK	O75643	4	11777.91	602.80
HLSDHLSELVEQTLSDLEQSK	O75643	3	11778.33	803.40
LELSVHLQPITR	O75643	3	6463.56	469.28
LTAIDILTTC(Methylthio)AADIQR	O75643	2	13199.51	882.46
LYDLNHNEIGELIR	O75643	3	7560.42	566.96
M(Oxidation)DTDLETM(Oxidation)DLDQGGEALAPR	O75643	2	6919.78	1105.48
M(Oxidation)TQNPNYYNLQGISHR	O75643	3	4206.52	651.31
MTQNPNYYNLQGISHR	O75643	3	4594.64	645.98
RLDLVHTAALMLDKNNLVK	O75643	4	8302.19	541.81
SGGPVVVLVQLEREEEVTGPVIAPLFPQK	O75643	3	12091.36	1029.91
SLQYEYK	O75643	2	2782.59	465.73
SLVQEMVGSFGK	O75643	2	8622.79	641.33
TGNFQVTELGR	O75643	2	4983.82	611.31
TNLLLQAHLSR	O75643	3	4683.05	422.58
TRRDEPTGEVLSLVGKLEGTR	O75643	4	7443.32	579.07
VPIPVKESIEEPSAK	O75643	3	4274.05	541.63
VVLLTGETSTDLK	O75643	2	6029.52	688.39
YAQAGFEGFK	O75643	2	4657.65	559.27
AHGGYSVFAGVGER	P06576	3	4066.84	469.57
AHGGYSVFAGVGER	P06576	2	4067.38	703.84
AIAELGIYPAVDPLDSTSR	P06576	2	10056.72	994.52
DQEGQDVLLFIDNIFR	P06576	2	13754.13	961.49
EGNDLYHEM(Oxidation)IESGVINLK	P06576	3	6967.34	693.00
EGNDLYHEMIESGVINLK	P06576	3	9519.98	687.67
ETRLVLEVAQHLGESTVR	P06576	4	7089.19	510.03
ETRLVLEVAQHLGESTVR	P06576	3	7085.92	679.71
FLSQPFQVAEVFTGHM(Oxidation)GK	P06576	3	8779.41	680.34
FLSQPFQVAEVFTGHMGK	P06576	3	9681.53	675.01
FLSQPFQVAEVFTGHM(Oxidation)GK	P06576	2	8779.66	1020.01
FTQAGSEVSALLGR	P06576	2	7458.45	718.38
FTQAGSEVSALLGRIPSAVGYQPTLATDM(Dioxidation)GTMQER	P06576	3	10274.31	1238.94
FTQAGSEVSALLGRIPSAVGYQPTLATDMGTM(Oxidation)QER	P06576	3	10761.70	1233.61
GFQQILAGEYDHLPEQAFYM(Oxidation)VGPIEEAVAK	P06576	3	11504.92	1122.88
GFQQILAGEYDHLPEQAFYMVGPIEEAVAK	P06576	3	12341.34	1117.55
GGKIGLFGGAGVGK	P06576	2	3908.14	609.35
GQKVLDSGAPIKIPVGPETLGR	P06576	4	6585.67	558.82
GQKVLDSGAPIKIPVGPETLGR	P06576	3	6587.37	744.76
GSITSVQAIYVPADDLTDPAPATTFAHLDATTVLSR	P06576	3	11298.03	1238.97
IGLFGGAGVGK	P06576	2	5844.10	488.28
IM(Oxidation)DPNIVGSEHYDVAR	P06576	3	4749.42	611.29
IM(Oxidation)DPNIVGSEHYDVAR	P06576	2	4748.42	916.44
IMDPNIVGSEHYDVAR	P06576	3	5605.08	605.96
IM(Oxidation)DPNIVGSEHYDVAR	P06576	3	5605.37	611.29
IMDPNIVGSEHYDVAR	P06576	2	5607.40	908.44
IM(Oxidation)NVIGEPIDER	P06576	2	5304.34	701.36
IMNVIGEPIDER	P06576	2	6546.60	693.36
IM(Oxidation)NVIGEPIDERGPIK	P06576	3	5343.69	599.66
IMNVIGEPIDERGPIK	P06576	3	6292.57	594.33
IM(Oxidation)NVIGEPIDERGPIK	P06576	3	6297.18	599.66
IMNVIGEPIDERGPIK	P06576	2	6296.13	890.98
IM(Oxidation)NVIGEPIDERGPIK	P06576	2	5333.90	898.98
IMNVIGEPIDERGPIKTK	P06576	4	5258.30	503.28
IM(Oxidation)NVIGEPIDERGPIKTK	P06576	4	4395.74	507.28
IM(Oxidation)NVIGEPIDERGPIKTK	P06576	3	4391.38	676.04
IM(Oxidation)NVIGEPIDERGPIKTK	P06576	4	5256.54	507.28
IPSAVGYQPTLATDM(Dioxidation)GTMQER	P06576	2	6010.84	1149.54
IPSAVGYQPTLATDMGTM(Oxidation)QER	P06576	2	7115.37	1141.54