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	100%
identified (total)	26,794	100%
identified (unique modified)	21,658	80.83%
identified (unique stripped)	19,580	73.08%

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.

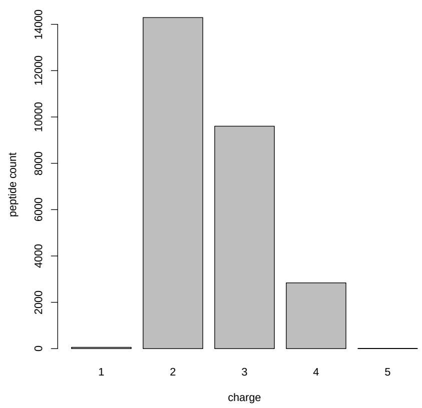


Figure 1: Charge distribution of peptide quantifications.

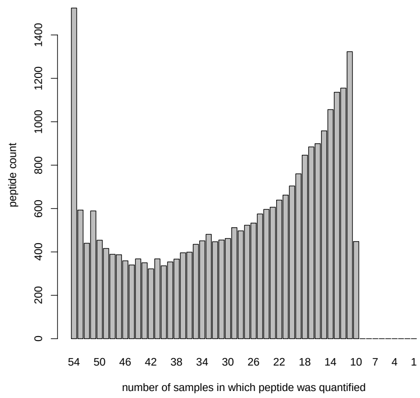


Figure 2: Frequency plot of peptide quantifications.

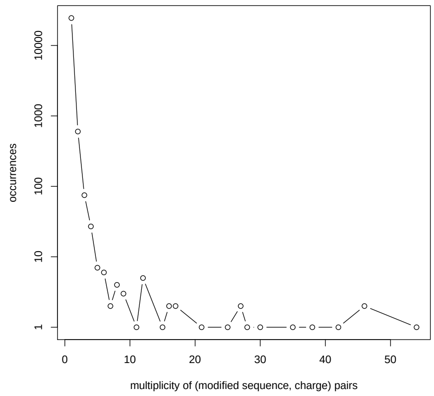


Figure 3: (modified sequence, charge) pair multiplicity vs frequency plot. Each peptide feature (characterised by a (possibly) modified peptide sequence and a charge state) should ideally occur only once in the analysis. In other words, peptides of multiplicity 1 should have a very high frequency. The plot below should show a significant spike on the left and can be used as QC of the analysis.

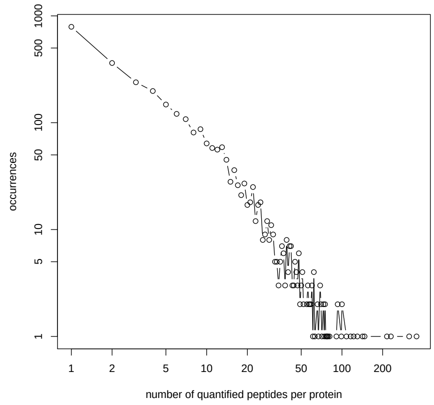


Figure 4: Number of quantified peptides per protein.

sample	finite	zero	nan
1	26794	0	0
2	26794	0	0
3	26794	0	0
4	26794	0	0
5	26794	0	0
6	26794	0	0
7	26794	0	0
8	26794	0	0
9	26794	0	0
10	26794	0	0
11	26794	0	0
12	26794	0	0
13	26794	0	0
14	26794	0	0
15	26794	0	0
16	26794	0	0
17	26794	0	0
18	26794	0	0
19	26794	0	0
20	26794	0	0
21	26794	0	0
22	26794	0	0
23	26794	0	0
24	26794	0	0
25	26794	0	0
26	26794	0	0
27	26794	0	0
28	26794	0	0
29	26794	0	0
30	26794	0	0
31	26794	0	0
32	26794	0	0
33	26794	0	0
34	26794	0	0
35	26794	0	0
36	26794	0	0
37	26794	0	0
38	26794	0	0
39	26794	0	0
40	26794	0	0
41	26794	0	0
42	26794	0	0
43	26794	0	0
44	26794	0	0
45	26794	0	0
46	26794	0	0
47	26794	0	0
48	26794	0	0
49	26794	0	0
50	26794	0	0
51	26794	0	0
52	26794	0	0
53	26794	0	0
54	26794	0	0

Table 3: Statistics of quantifications.

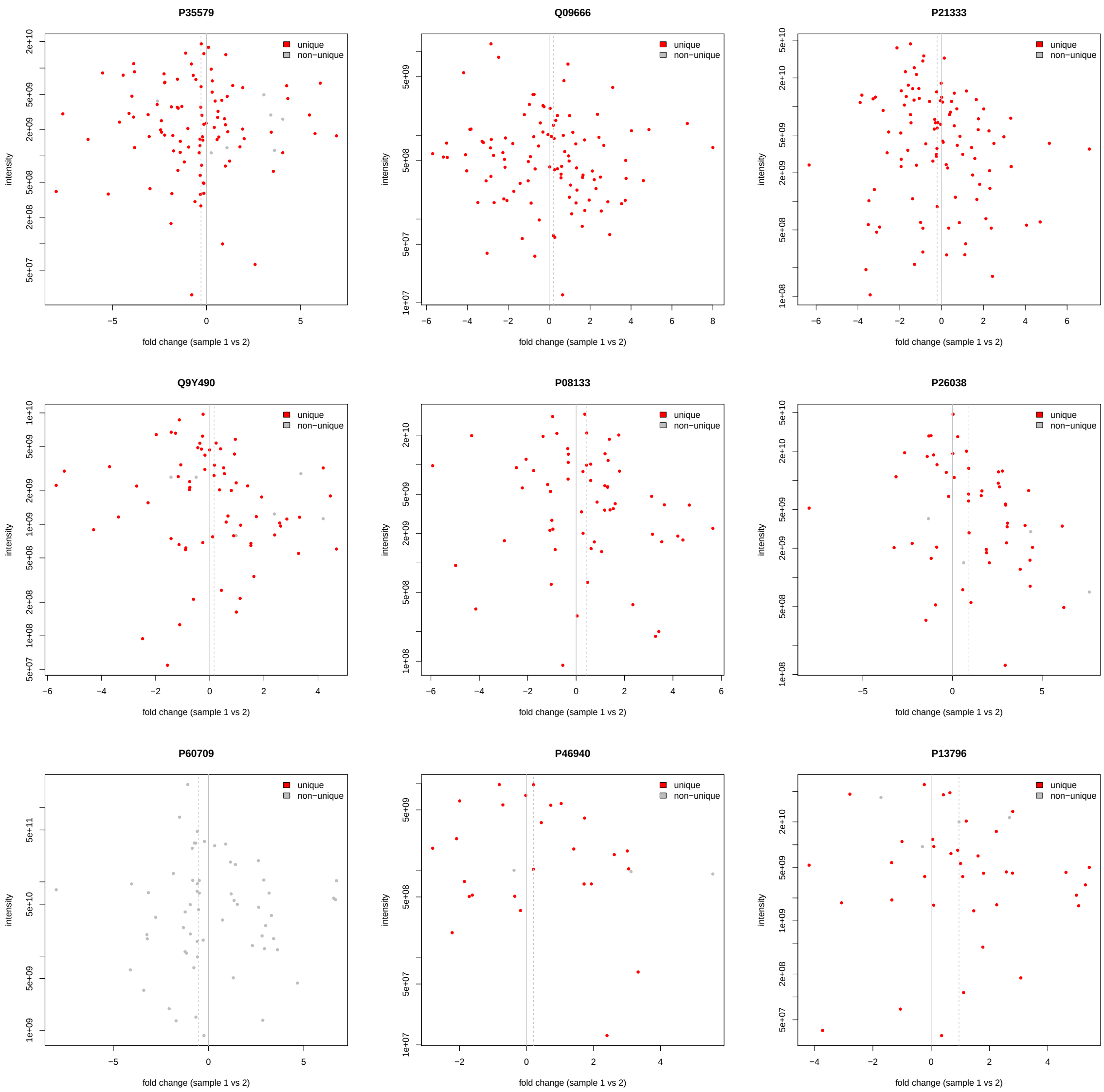
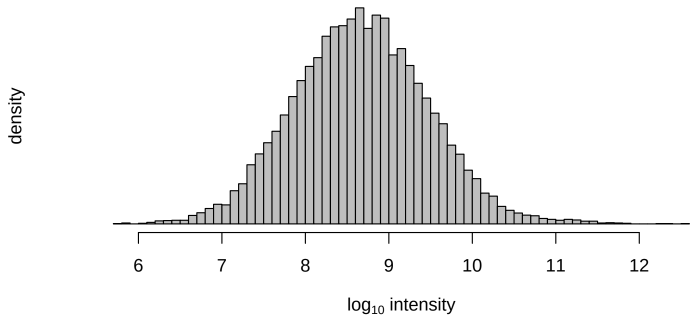
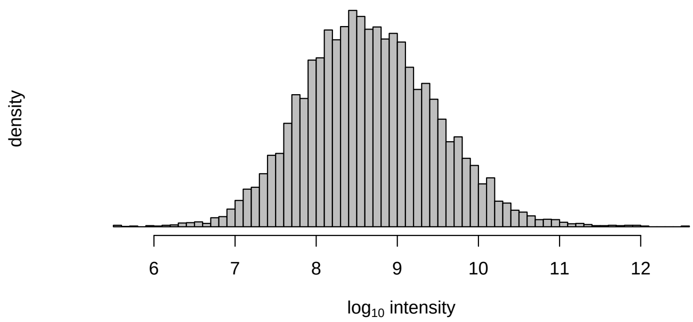


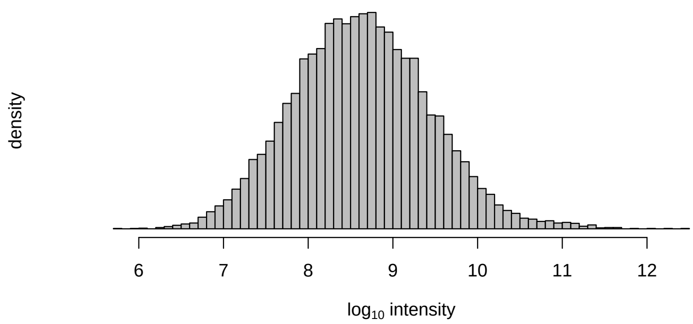
Figure 5: Fold changes of peptide abundances 1 and 2. For proteins with the largest number of quantified peptides.



(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 6: peptide abundance distributions.

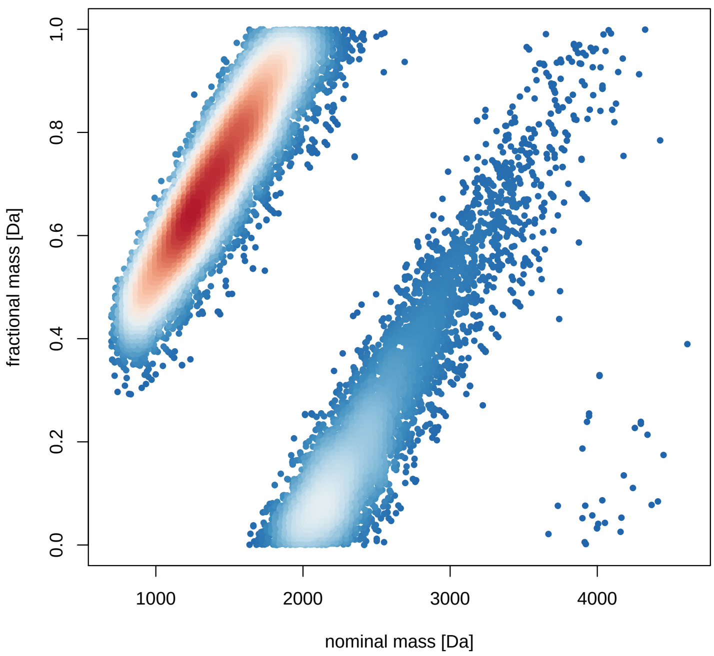


Figure 7: Kendrick nominal fractional mass plot

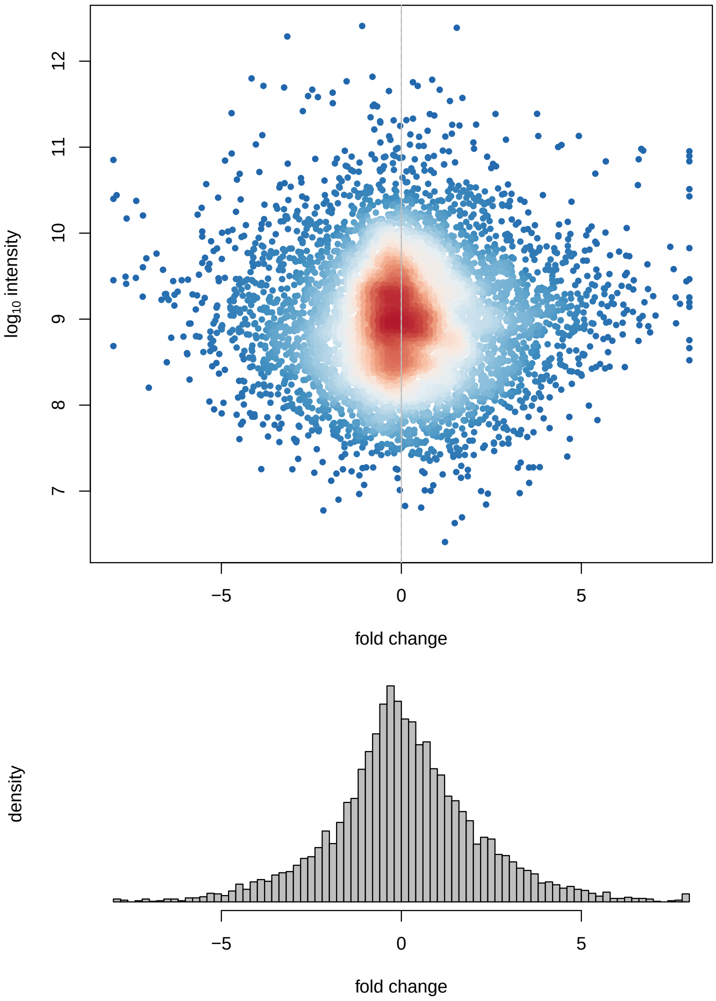


Figure 8: Fold changes of peptide abundances 1 and 2.
median(fc) $= -0.0026$ sd(fc) $= 2.0776$

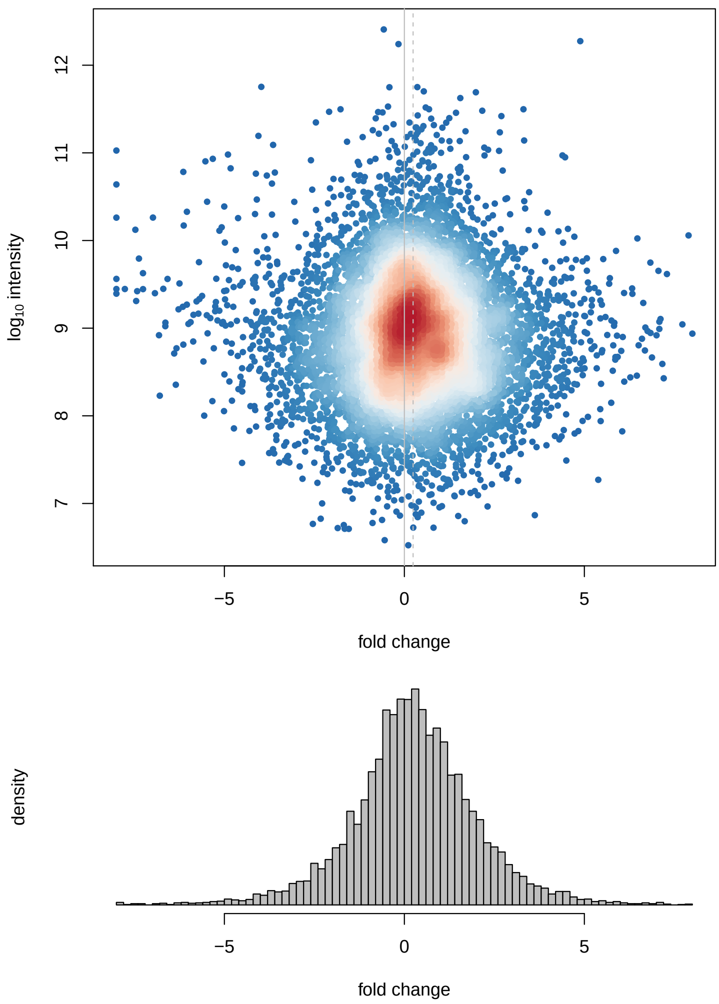


Figure 9: Fold changes of peptide abundances 1 and 3.
median(fc) = 0.2421   sd(fc) = 1.7661

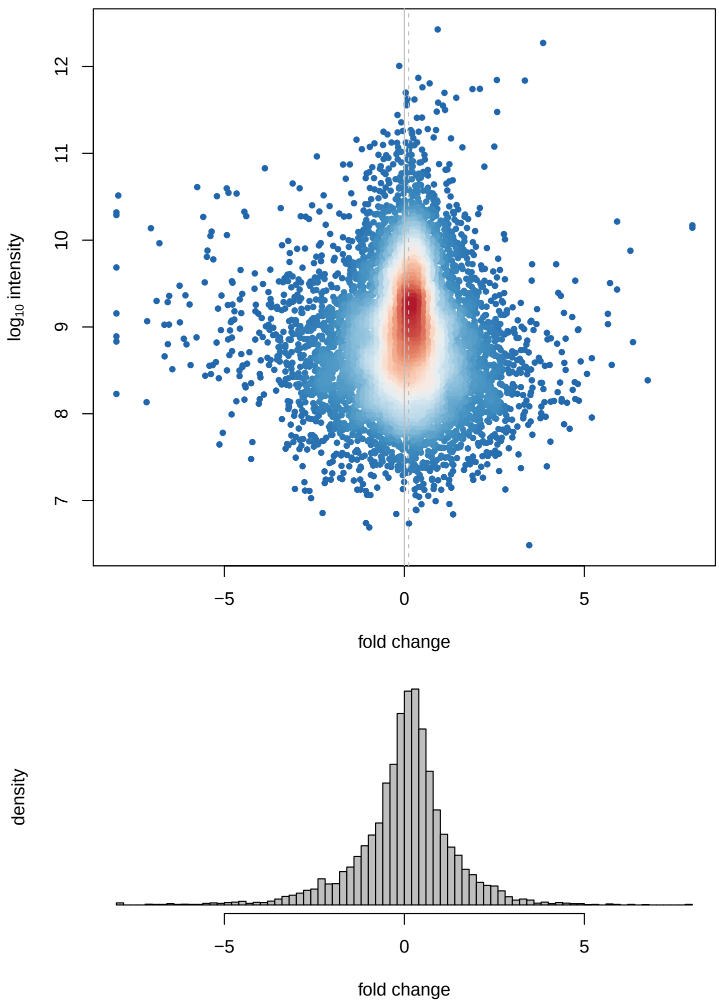


Figure 10: Fold changes of peptide abundances 2 and 3.
median(fc) = 0.1175   sd(fc) = 1.3543

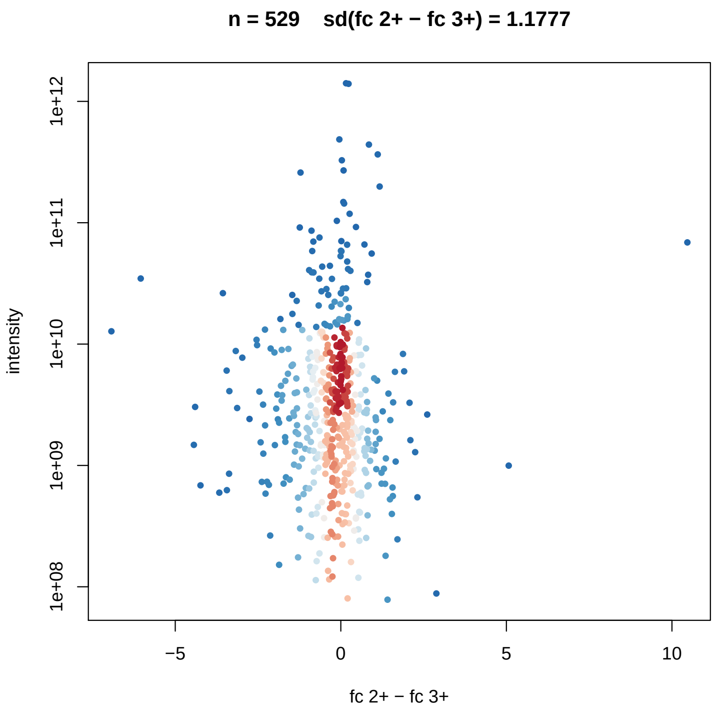


Figure 11: Fold changes of the same peptide in charge 2+ and 3+ are expected to be identical. Here we plot the difference of the 2+ and 3+ fold changes of sample 1 vs. sample 2 of all peptides which were identified and quantified in both charge states.

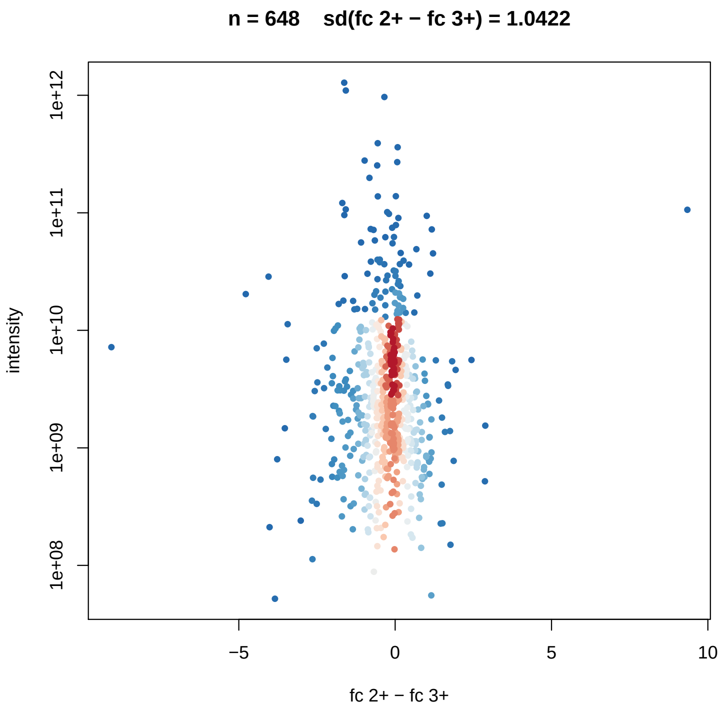


Figure 12: Fold changes of the same peptide in charge 2+ and 3+ are expected to be identical. Here we plot the difference of the 2+ and 3+ fold changes of sample 1 vs. sample 3 of all peptides which were identified and quantified in both charge states.

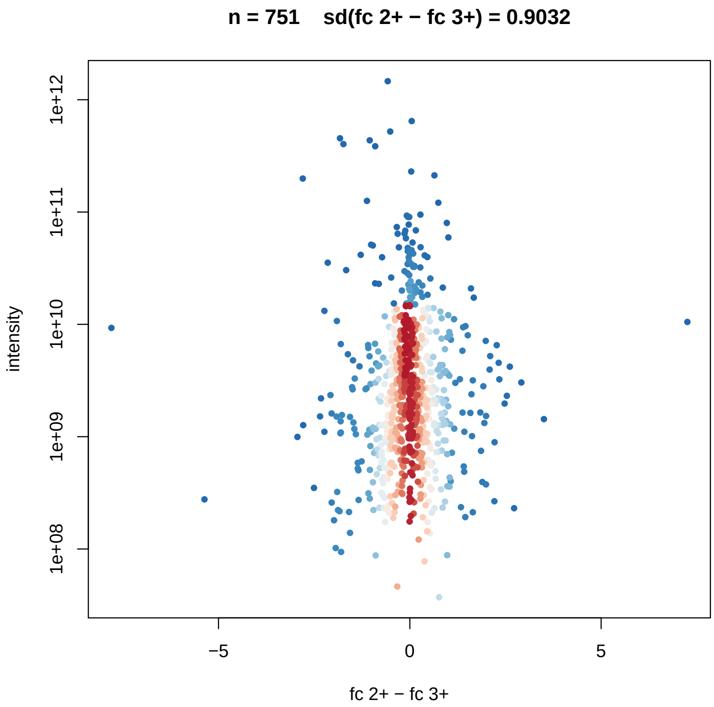


Figure 13: Fold changes of the same peptide in charge 2+ and 3+ are expected to be identical. Here we plot the difference of the 2+ and 3+ fold changes of sample 2 vs. sample 3 of all peptides which were identified and quantified in both charge states.

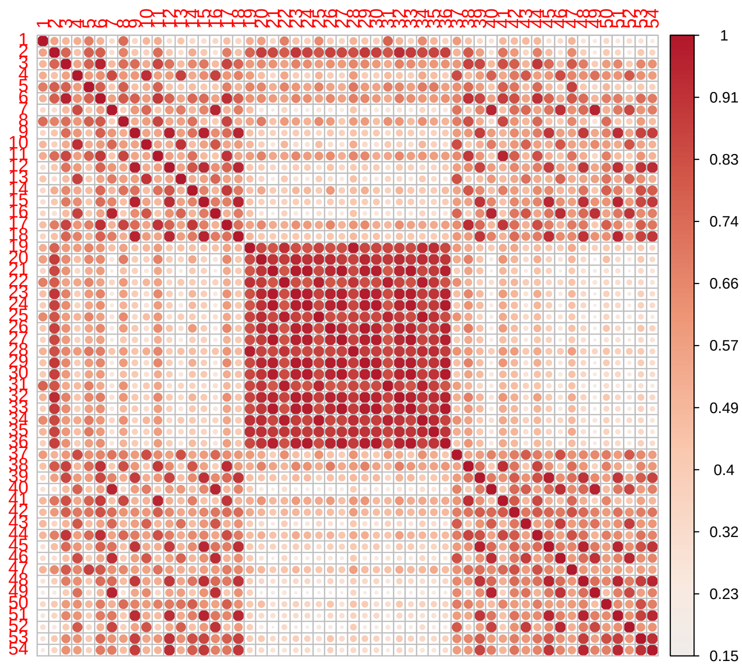


Figure 14: Pearson correlation of all peptide abundances. (min correlation = 0.1484, median correlation = 0.5701, max correlation = 1)

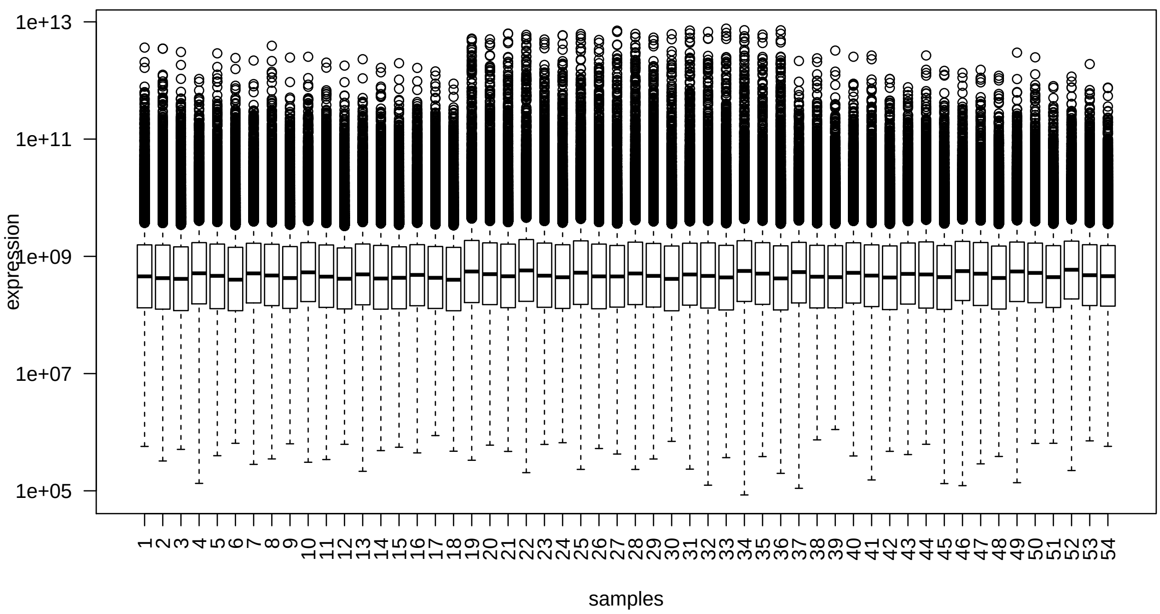


Figure 15: Boxplot of all peptide abundances.

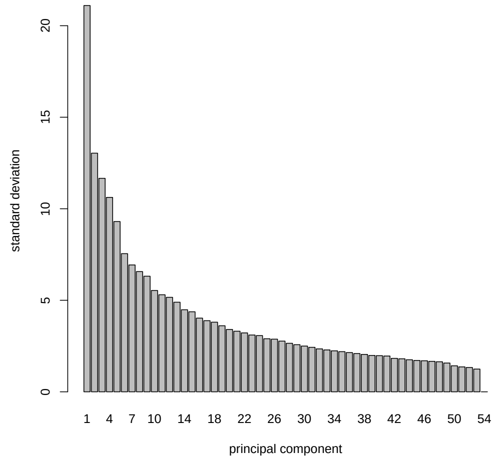


Figure 16: Standard deviation of all principal components.

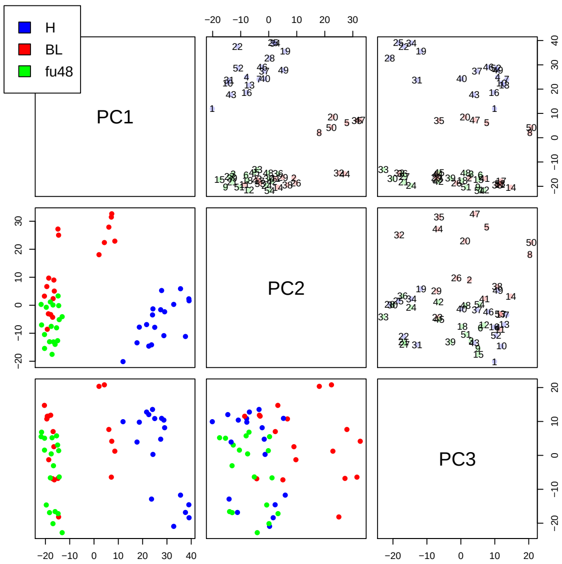


Figure 17: Principal Component Analysis of all peptides with complete quantifications. Any peptides with one or more missing values are ignored. The numbers in the upper right panels correspond to the sample IDs.

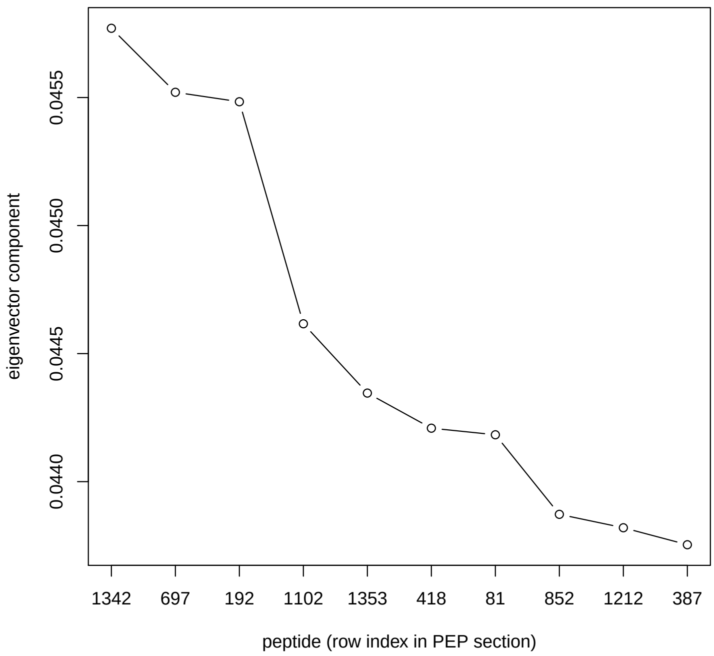


Figure 18: Most important contributions to the first principal component.

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 4: Most important contributions to the first principal component.

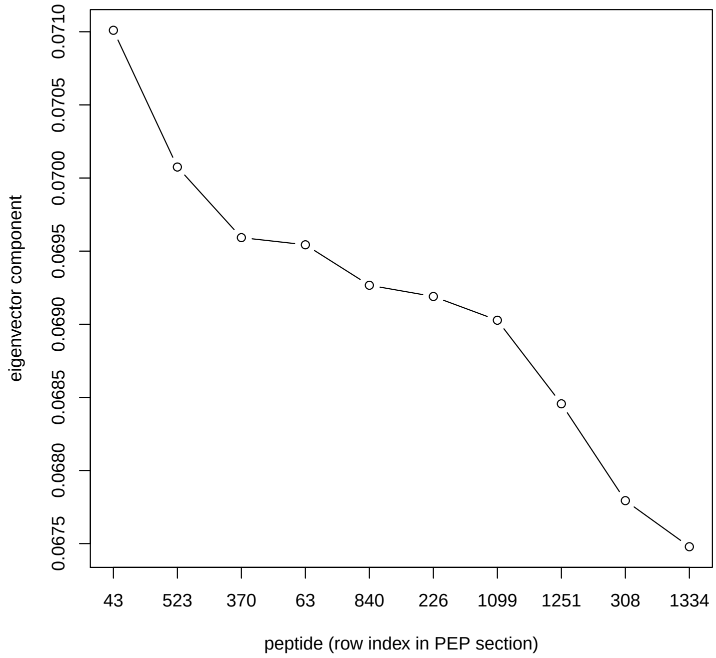


Figure 19: Most important contributions to the second principal component.

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 5: Most important contributions to the second principal component.

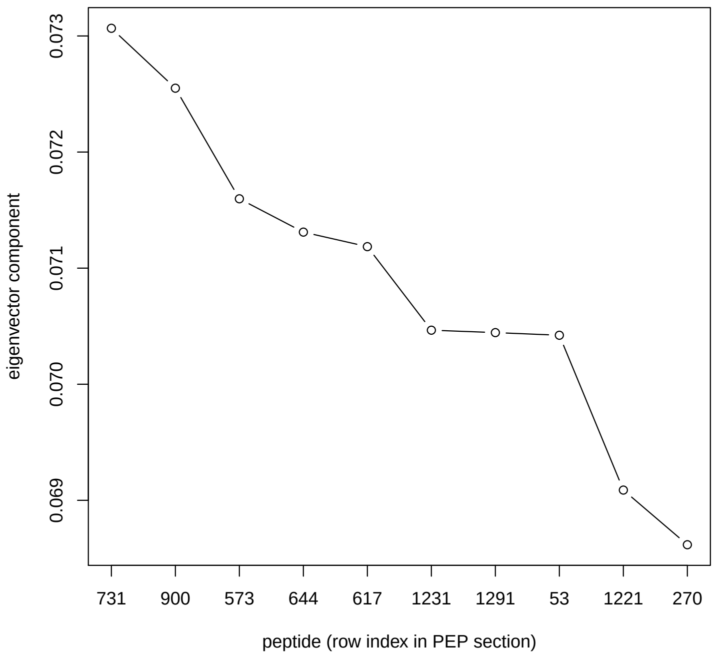


Figure 20: Most important contributions to the third principal component.

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 6: Most important contributions to the third principal component.

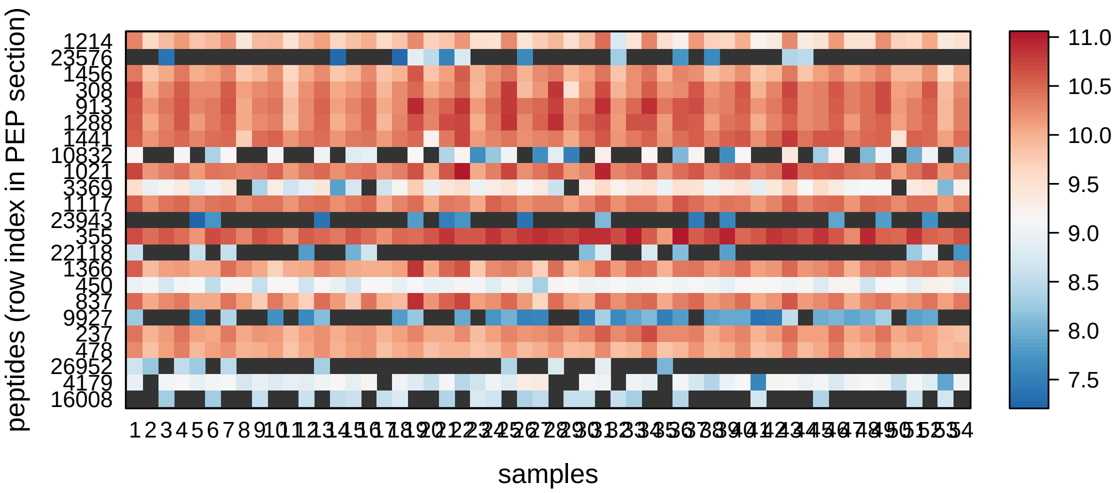


Figure 21: Logarithmic peptide abundances for all peptides of interest.

row index	modified sequence	accession	charge	retention time	m/z
1214	SSAAPPPPPR(Label:13C(6)15...	STD_01	2	1659.92	493.77
23576	SSAAPPPPPR(Label:13C(6)15...	STD_01	2	1605.04	493.76
1456	GISNEGQNASIK(Label:13C(6)...	STD_02	2	2041.39	613.32
308	HVLTSIGEK(Label:13C(6)15N...	STD_03	2	2127.71	496.29
913	DIPVPK(Label:13C(6)15N(2)...	STD_04	2	2653.71	451.28
1288	IGDYAGIK(Label:13C(6)15N(...	STD_05	2	3096.71	422.74
1441	TASEFDSAIAQDK(Label:13C(6...	STD_06	2	4266.53	695.83
10832	TASEFDSAIAQDK	STD_06	2	4271.48	691.83
1021	SAAGAFGPELSR(Label:13C(6)...	STD_07	2	4457.27	586.80
3369	SAAGAFGPELSR(Label:13C(6)...	STD_07	2	4650.67	586.80
1117	ELGQSGVDTYLQTK(Label:13C(...	STD_08	2	5741.14	773.90
23943	ELGQSGVDTYLQTK(Label:13C(...	STD_08	2	5880.07	773.90
355	GLILVGGYGTR(Label:13C(6)1...	STD_09	2	6431.53	558.33
22118	GLILVGGYGTR(Label:13C(6)1...	STD_09	2	4427.35	558.33
1366	GILFVGSGVSGGEEGAR(Label:1...	P52209	2	6781.34	801.41
450	GILFVGSGVSGGEEGAR	P52209	2	6780.92	796.41

837	SFANQPLEVVYSK(Label:13C(6...	STD_11	2	6787.30	745.39
9927	SFANQPLEVVYSK(Label:13C(6...	STD_11	2	6606.62	745.39
237	LTILEELR(Label:13C(6)15N(...	STD_12	2	7538.66	498.80
478	ELASGLSFPVGFK(Label:13C(6...	STD_14	2	9083.08	680.37
26952	ELASGLSFPVGFK(Label:13C(6...	STD_14	2	8764.02	680.37
4179	LSSEAPALFQFDLK(Label:13C(...	STD_15	2	9657.05	787.42
16008	AKGILFVGSGVSGGEEGAR	P52209	3	4941.74	597.65

Table 7: 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.

row index	modified sequence	accession	charge	retention time	m/z
5	DYLHLPPEIVPATLRR	P46783	3	8103.29	630.69
1721	KAEAGAGSATEFQFR	P46783	2	3516.88	785.39
2475	AEAGAGSATEFQFR	P46783	2	5036.50	721.34
2584	KAEAGAGSATEFQFR	P46783	3	3518.31	523.93
3119	IAIYELLFK	P46783	2	10732.68	555.33
3411	DYLHLPPEIVPATLRR	P46783	4	8100.98	473.27
5284	DYLHLPPEIVPATLR	P46783	3	9558.62	578.66
8795	SAVPPGADKKAEAGAGSATEFQFR	P46783	4	4302.34	598.80
9684	SAVPPGADKKAEAGAGSATEFQFR	P46783	3	4302.30	798.07
10741	GYVKEQFAWR	P46783	3	4253.53	428.56
11596	IAIYELLFKEGVM(Oxidation)V...	P46783	3	10197.44	614.01
15136	HFYWYLTNEGIQYLR	P46783	3	9290.39	668.33
15766	GYVKEQFAWR	P46783	2	4257.40	642.33
19976	DYLHLPPEIVPATLR	P46783	2	9548.91	867.48
20490	HPELADKNVPNLHVM(Oxidation...	P46783	4	2806.75	465.25
25208	SRPETGRPRPK	P46783	2	1112.69	640.86
26010	SRPETGRPRPK	P46783	3	1112.97	427.58
2595	LTIHAPPQELGPPVQR	P12270	3	5244.98	585.00
4982	NLQEQTVQLQSELSR	P12270	2	6830.64	886.96
5219	TLSSVQNEVQEALQR	P12270	2	7739.83	851.44
5886	ISTQLDFASK	P12270	2	4987.08	555.30
11076	LSQELEYLTEDVKR	P12270	3	6542.97	574.97
11273	GIASTSDPPTANIKPTPVVSTPSK	P12270	3	4902.51	789.09
11949	FKVESEQQYFEIEKR	P12270	3	4954.28	654.00
13013	RPSTSQTVSTPAPVPVIESTEAIEA...	P12270	3	6727.12	899.14
13171	LENEVEQR	P12270	2	1693.68	508.75
13646	LESALTELEQLRK	P12270	3	6908.25	510.62
13673	YLDEIVKEVEAK	P12270	3	7196.92	479.26
14084	LSSQIEKLEHEISHLK	P12270	4	6322.55	473.51
14534	GQNLLLTNLQTIQGILER	P12270	2	12445.40	1012.58
14775	NLDVQLLDTK	P12270	2	6805.16	579.82
15566	LLSEKEVHTK	P12270	2	1506.47	592.33
15882	EKEIAETRFEVAQVESLR	P12270	3	5813.97	712.04
17342	ILLSQTTGVAIPLHASSLDDVSLAS...	P12270	3	9456.43	945.52
18730	FLADQQSEIDGLKGRHEK	P12270	4	3196.05	518.52
20518	KLELDILPLQEANAELSEK	P12270	3	9473.26	718.40
22013	EKGNEILELK	P12270	2	3452.76	586.83
22088	LQEQVTDLR	P12270	2	3580.96	551.30
23121	TKEELEAEKR	P12270	2	1216.40	616.83
23610	EGVQGPLNVSLSEEGKSQEQILEIL...	P12270	3	10181.28	951.51
24602	SAADDSEAKSNELTR	P12270	3	1865.12	531.92
25260	ITELQLKLESALTELEQLRK	P12270	4	10747.62	589.59
26016	AALKQLQEIFENYKK	P12270	4	6949.96	456.51

26106	SQEQILEILR	P12270	2	7860.87	614.85
26244	AADSQNSGEGNTGAAESSFSQEVSR	P12270	2	4519.04	1243.53
26421	SAADDSEAKSNELTR	P12270	2	1834.45	797.37
26635	KLENEVEQR	P12270	2	1635.88	572.80

Table 8: Proteins of interest.

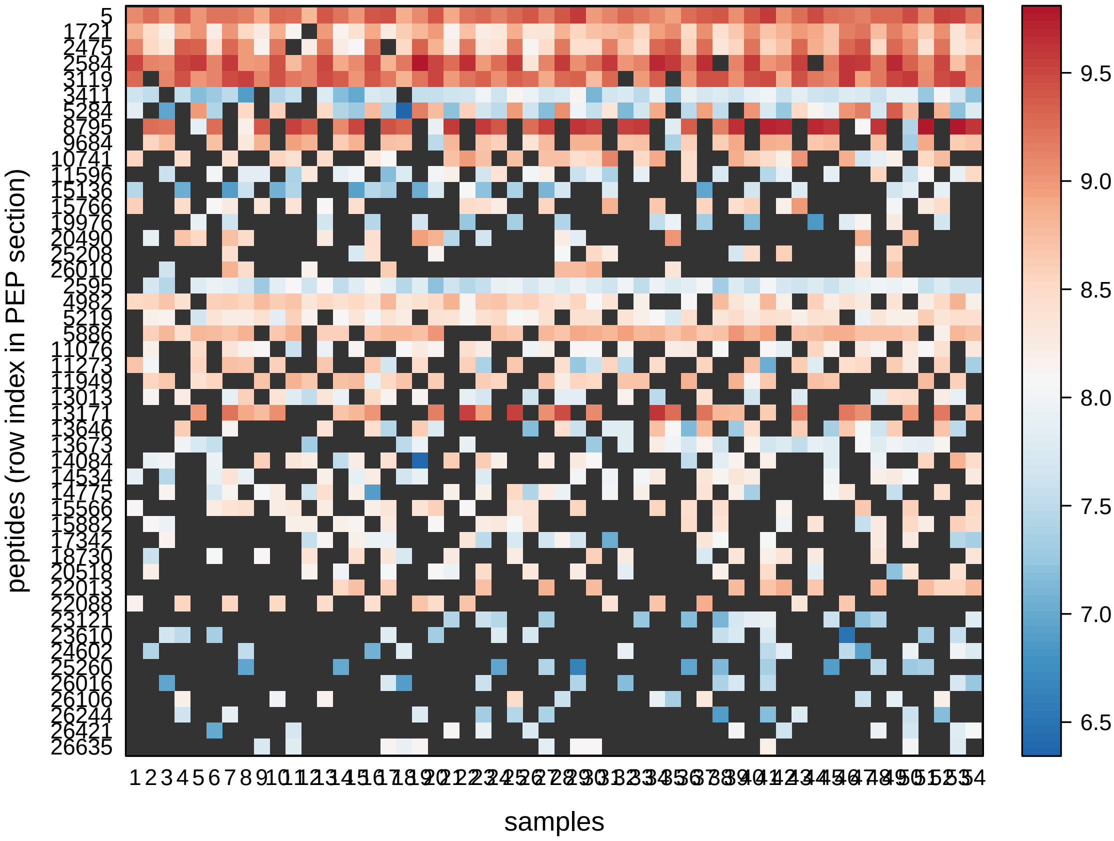


Figure 22: Logarithmic peptide abundances for all proteins of interest.

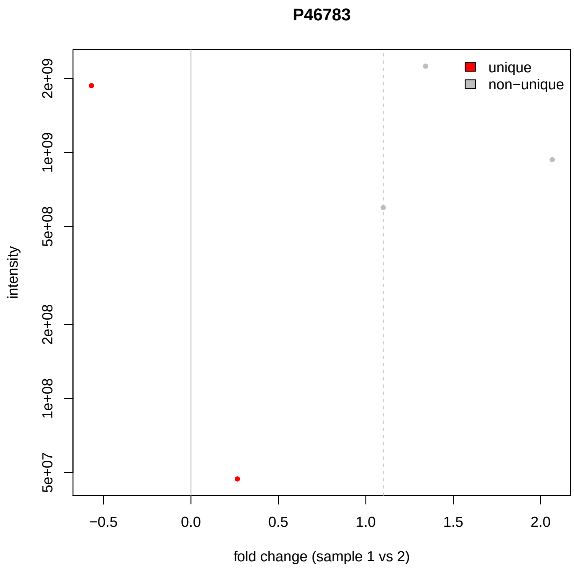


Figure 23: Fold changes of peptide abundances 1 and 2 for first protein of interest.

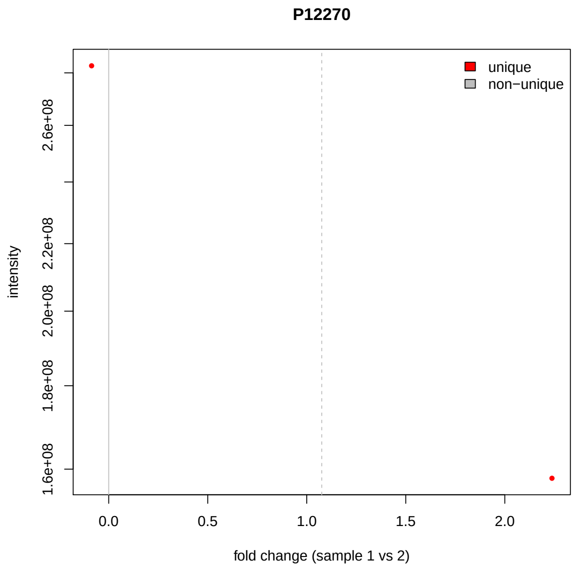


Figure 24: Fold changes of peptide abundances 1 and 2 for second protein of interest.