

Report for PEP Section in mzTab File example_6

The PEP section of the **mzTab** file contains 22,310 quantified peptide features measured in 2 samples.

	number of peptides	
quantified	22,310	100%
identified (total)	22,310	100%
identified (unique modified)	9,807	43.96%
identified (unique stripped)	8,214	36.82%

Table 1: Total number of quantified and identified peptides.

mod	specificity	number
Carbamidomethyl	C	4611
Label:13C(6)	K	3957
Label:13C(6)	R	2625

Table 2: Statistics of modifications.

sample	finite	zero	nan
1	21334	976	0
2	17514	4796	0

Table 3: Statistics of quantifications.

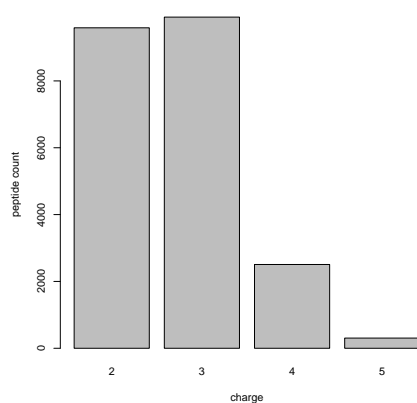


Figure 1: Charge distribution of peptide quantifications.

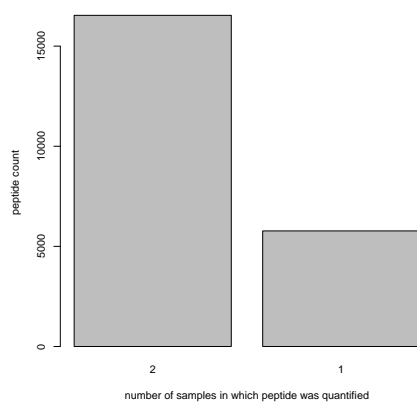


Figure 2: Frequency plot of peptide quantifications.

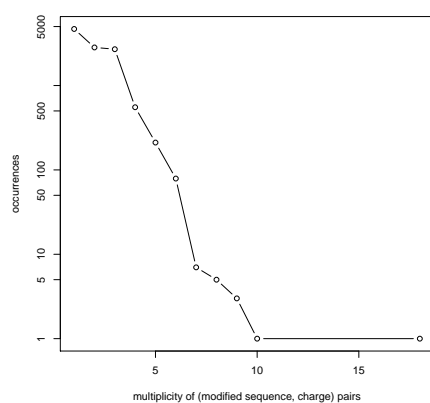


Figure 3: (modified sequence, charge) pair multiplicity vs frequency plot. Each peptide feature (characterised by a (possibly) modified peptide sequence and a charge state) should ideally occur only once in the analysis. In other words, peptides of multiplicity 1 should have a very high frequency. The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

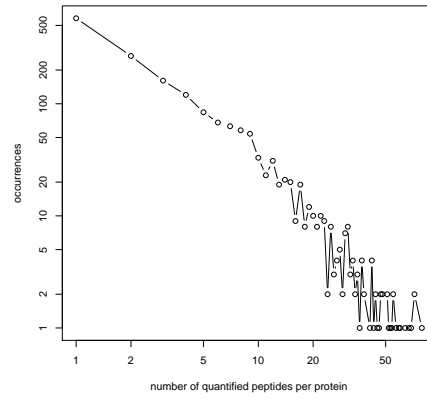


Figure 4: Number of quantified peptides per protein.

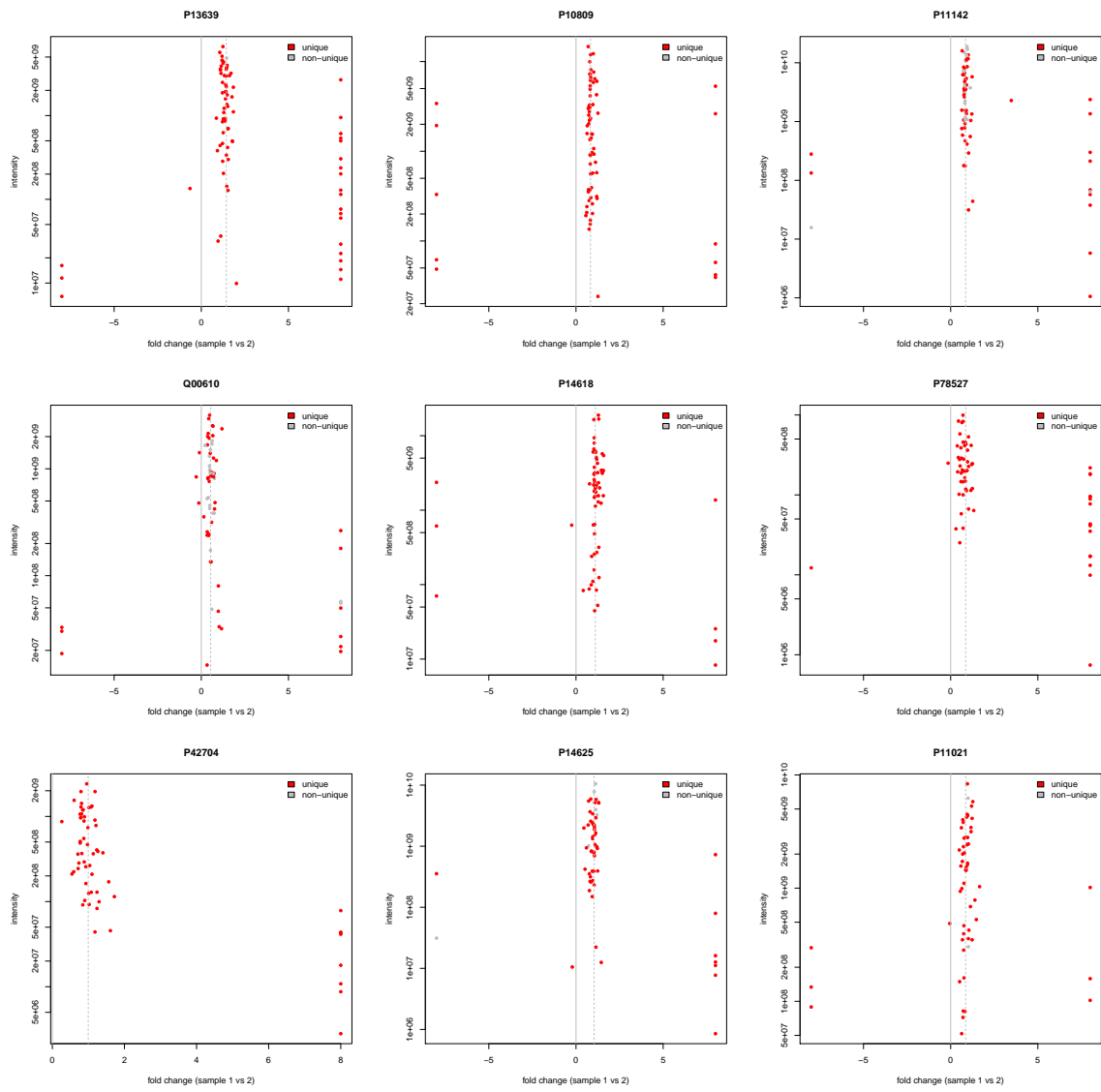
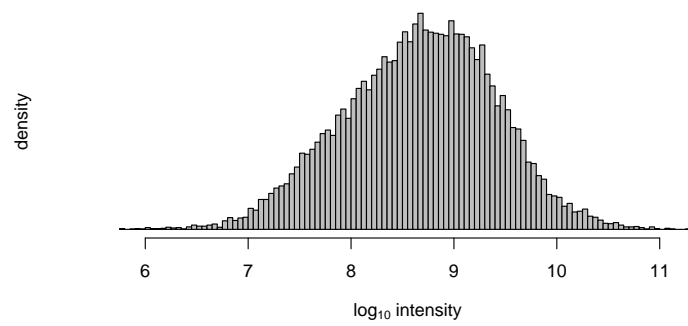
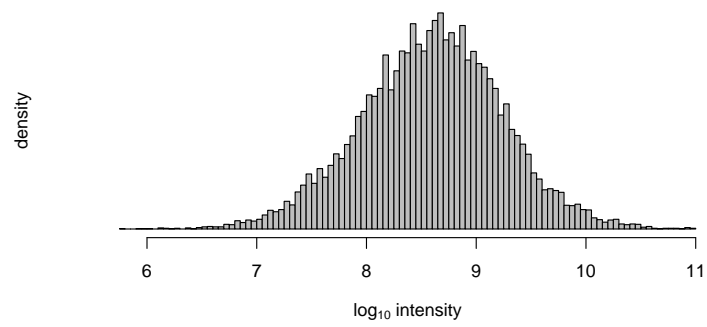


Figure 5: Fold changes of peptide abundances 1 and 2. For proteins with the largest number of quantified peptides.



(a) peptide abundances 1, median(intensity) = 454,615,008



(b) peptide abundances 2, median(intensity) = 243,896,504

Figure 6: peptide abundance distributions.

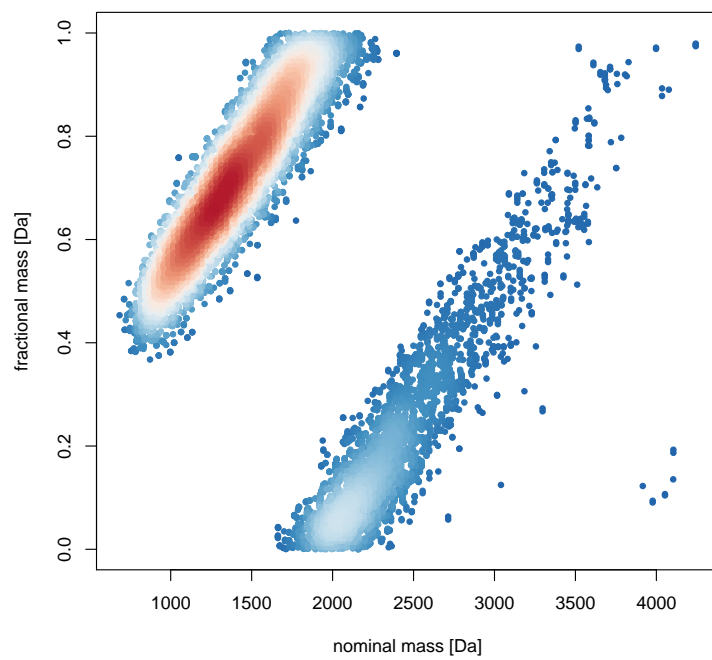


Figure 7: Kendrick nominal fractional mass plot

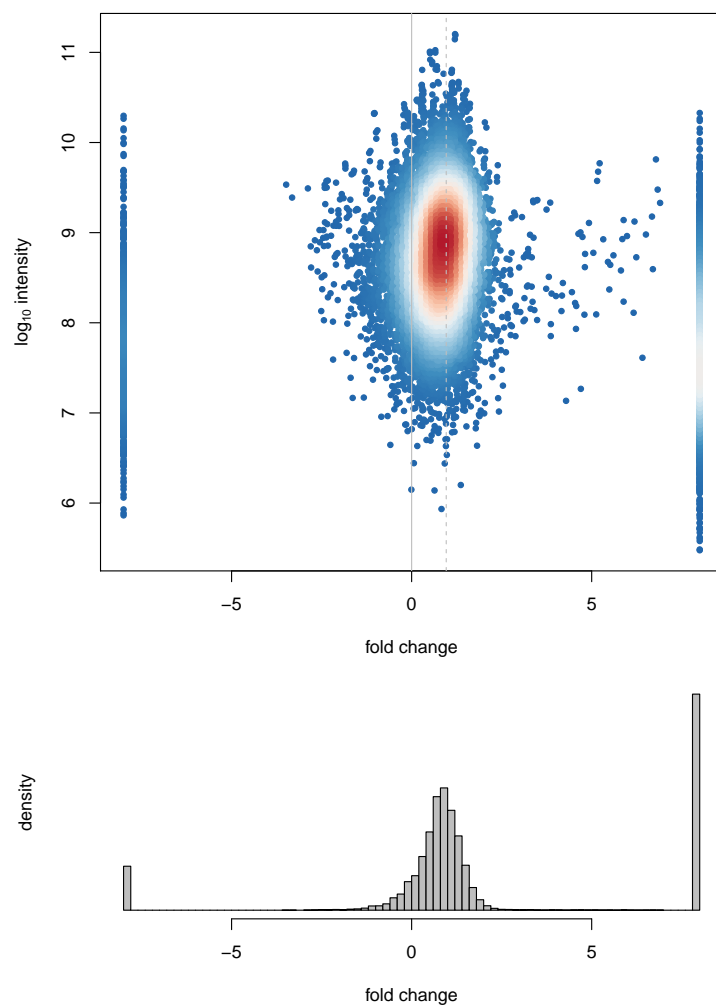


Figure 8: Fold changes of peptide abundances 1 and 2.
 $\text{median}(\text{fc}) = 0.9609$ $\text{sd}(\text{fc}) = 3.6836$

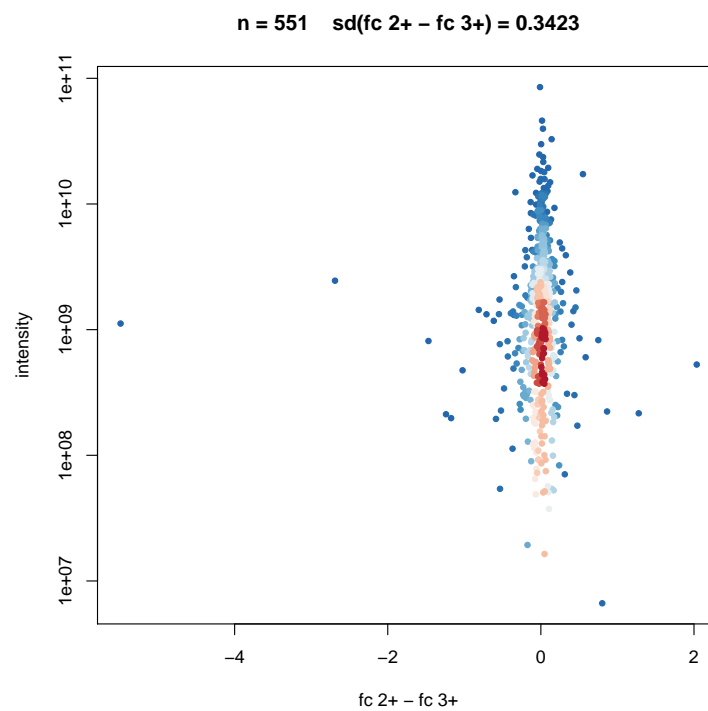


Figure 9: Fold changes of the same peptide in charge 2+ and 3+ are expected to be identical. Here we plot the difference of the 2+ and 3+ fold changes of sample 1 vs. sample 2 of all peptides which were identified and quantified in both charge states.

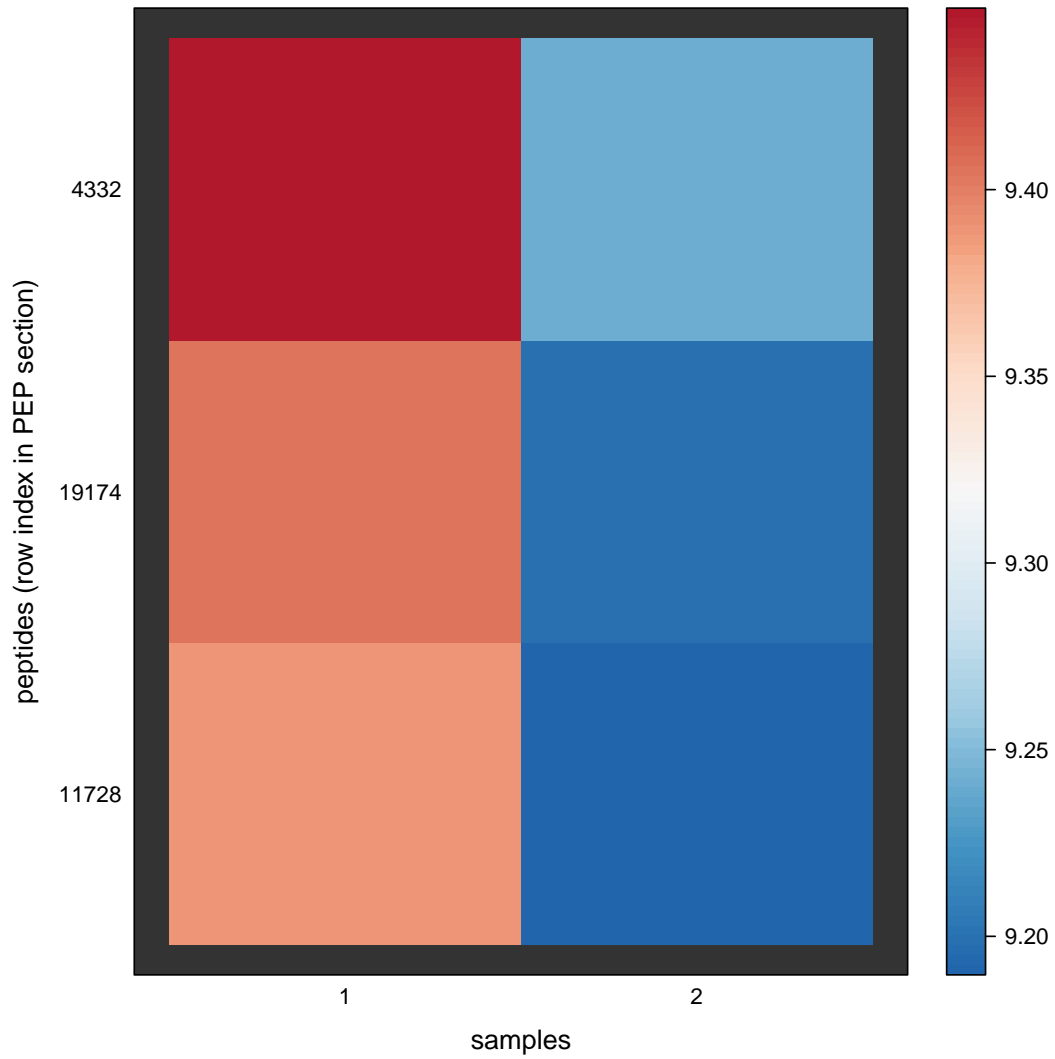


Figure 10: Logarithmic peptide abundances for all peptides of interest.

row index	modified sequence	accession	charge	retention time	m/z
4332	GILFVGSGVSGGEEGAR	P52209	2	2334.78	796.41
19174	GILFVGSGVSGGEEGAR	P52209	2	2335.85	796.41
11728	GILFVGSGVSGGEEGAR	P52209	2	2335.49	796.41

Table 4: 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
14127	IAIYELLFK	P46783	2	3767.59	555.33
6755	IAIYELLFK	P46783	2	3772.74	555.33
21653	IAIYELLFK	P46783	2	3770.19	555.33
9363	HPELADKNVPSNLHVMK	P46783	4	1355.06	461.25
2002	KAEAGAGSATEFQFR	P46783	3	1385.40	523.93
16849	KAEAGAGSATEFQFR	P46783	3	1391.61	523.93

9428	KAEAGAGSATEFQFR	P46783	3	1387.19	523.93
16806	HPELADKNVPNLHVMK	P46783	4	1369.56	461.25
1938	HPELADKNVPNLHVMK	P46783	4	1356.00	461.25
13450	DYLHLPPEIVPATLR	P46783	3	3288.28	578.66
16052	NVPNLHVMK	P46783	3	1030.46	351.20
20332	DYLHLPPEIVPATLRR	P46783	4	2891.25	473.27
1999	KAEAGAGSATEFQFR	P46783	2	1384.54	785.39
8586	NVPNLHVMK	P46783	3	1021.79	351.20
12851	DYLHLPPEIVPATLRR	P46783	4	2888.02	473.27
9422	KAEAGAGSATEFQFR	P46783	3	1382.02	523.93
9426	KAEAGAGSATEFQFR	P46783	2	1386.17	785.39
16851	KAEAGAGSATEFQFR	P46783	2	1392.91	785.39
14761	GQNLLLTNLQTIQGILER	P12270	3	4285.16	675.39
22267	GQNLLLTNLQTIQGILER	P12270	3	4285.98	675.39
7378	GQNLLLTNLQTIQGILER	P12270	3	4293.51	675.39
303	LSDK(Label:13C(6))VVASVK(...	P12270	3	650.82	349.21
7726	LSDKVVASVK	P12270	3	645.78	349.21
945	NIEELQQQNQR	P12270	2	929.09	700.36
3157	NLDVQLLDTKR	P12270	3	1847.85	438.92

Table 5: Proteins of interest.

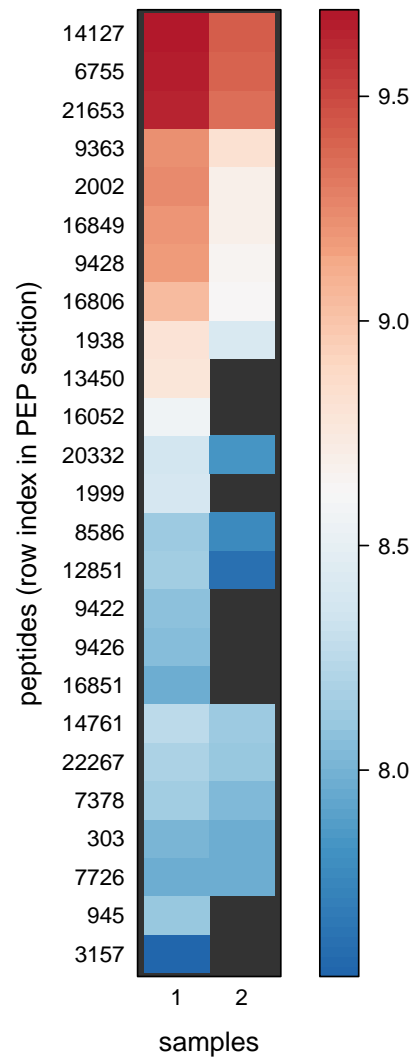


Figure 11: Logarithmic peptide abundances for all proteins of interest.

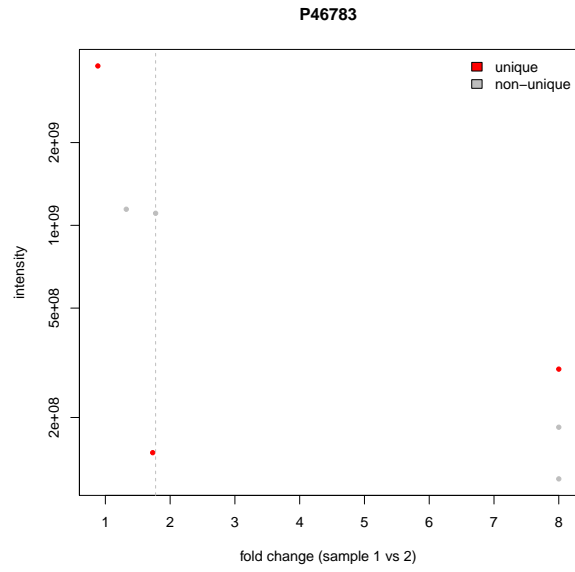


Figure 12: Fold changes of peptide abundances 1 and 2 for first protein of interest.

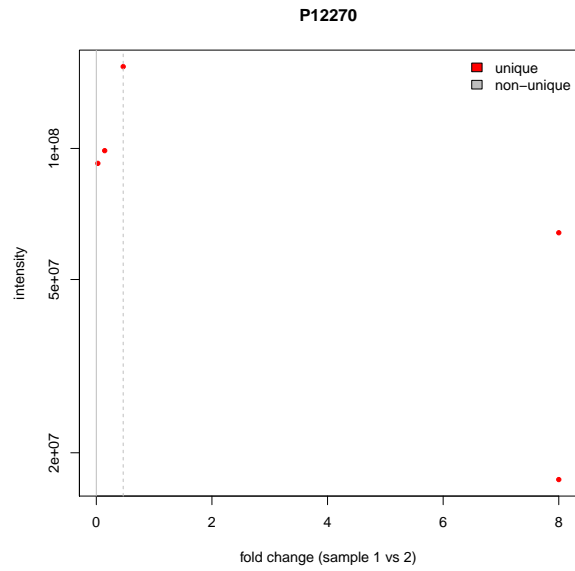


Figure 13: Fold changes of peptide abundances 1 and 2 for second protein of interest.