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.

modified sequence	accession	charge	retention time	m/z
SSAAPPPPPR(Label:13C(6)15N(4))	STD_01	2	1659.92	493.77
HVLTSIGEK(Label:13C(6)15N(2))	STD_03	2	2127.71	496.29
IGDYAGIK(Label:13C(6)15N(2))	STD_05	2	3096.71	422.74
TASEFDSAIAQDK(Label:13C(6)15N(2))	STD_06	2	4266.53	695.83
SAAGAFGPELSR(Label:13C(6)15N(4))	STD_07	2	4457.27	586.80
ELGQSGVDTYLQTK(Label:13C(6)15N(2))	STD_08	2	5741.14	773.90
GLILVGGYGTR(Label:13C(6)15N(4))	STD_09	2	6431.53	558.33
GILFVGSGVSGGEEGAR	P52209	2	6780.92	796.41
GILFVGSGVSGGEEGAR(Label:13C(6)15N(4))	P52209	2	6781.34	801.41
SFANQPLEVVYSK(Label:13C(6)15N(2))	STD_11	2	6787.30	745.39
ELASGLSFPVGFK(Label:13C(6)15N(2))	STD_14	2	9083.08	680.37

Table 2: 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
INQEELASGTPPARFPK	O15117	3	4675.29	618.99

Table 3: Proteins of interest.

modifications statistics

| mod	specificity	number
Oxidation	M	179
Methylthio	C	150
Label:13C(6)15N(2)	K	6
Label:13C(6)15N(4)	R	4

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.
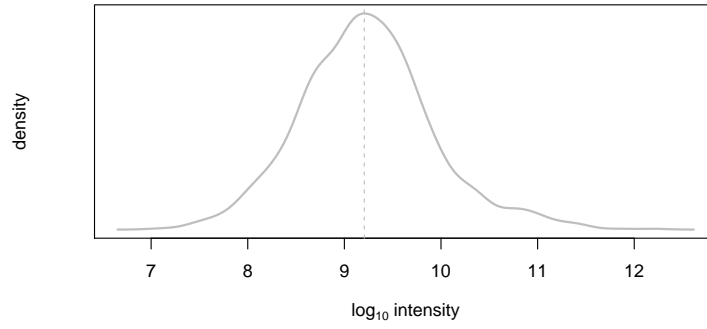
(a) peptide abundances 1, median(intensity) = 1, 605, 469, 952
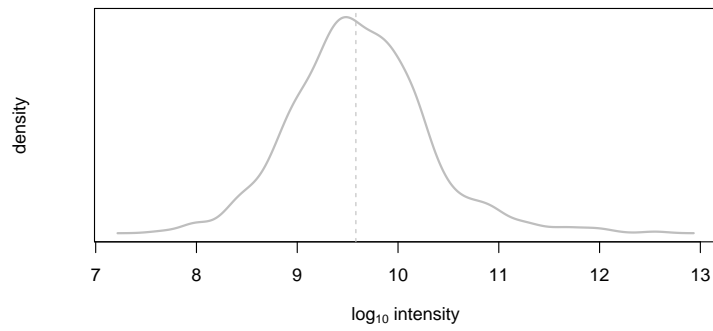
(b) peptide abundances 2, median(intensity) = 3, 819, 539, 968
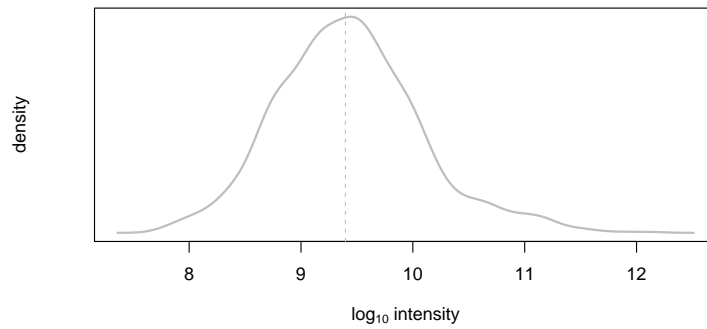
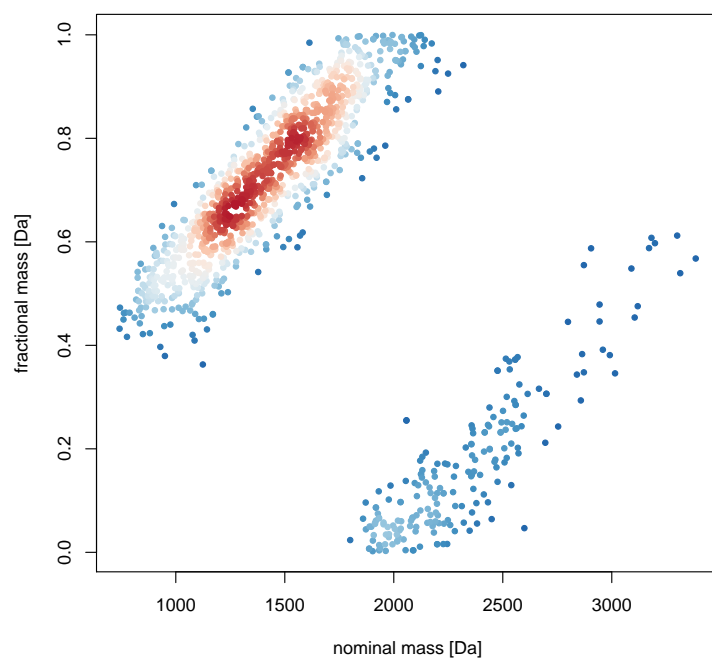(c) peptide abundances 3, median(intensity) = 2, 497, 959, 936

Figure 3: peptide abundance distributions.
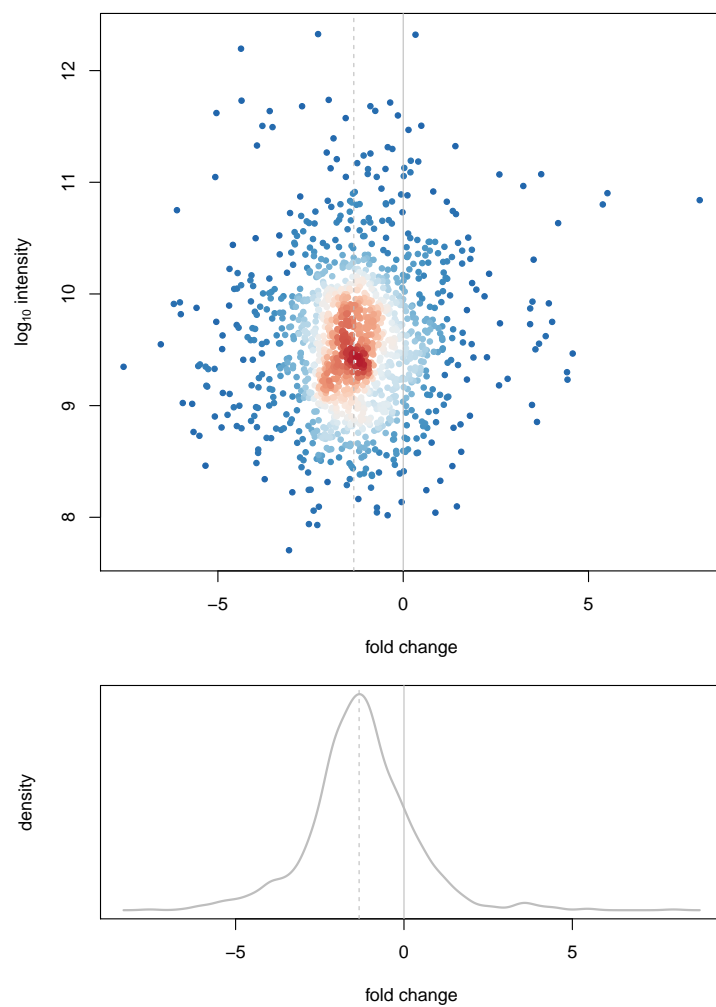
Figure 4: Kendrick nominal fractional mass plot

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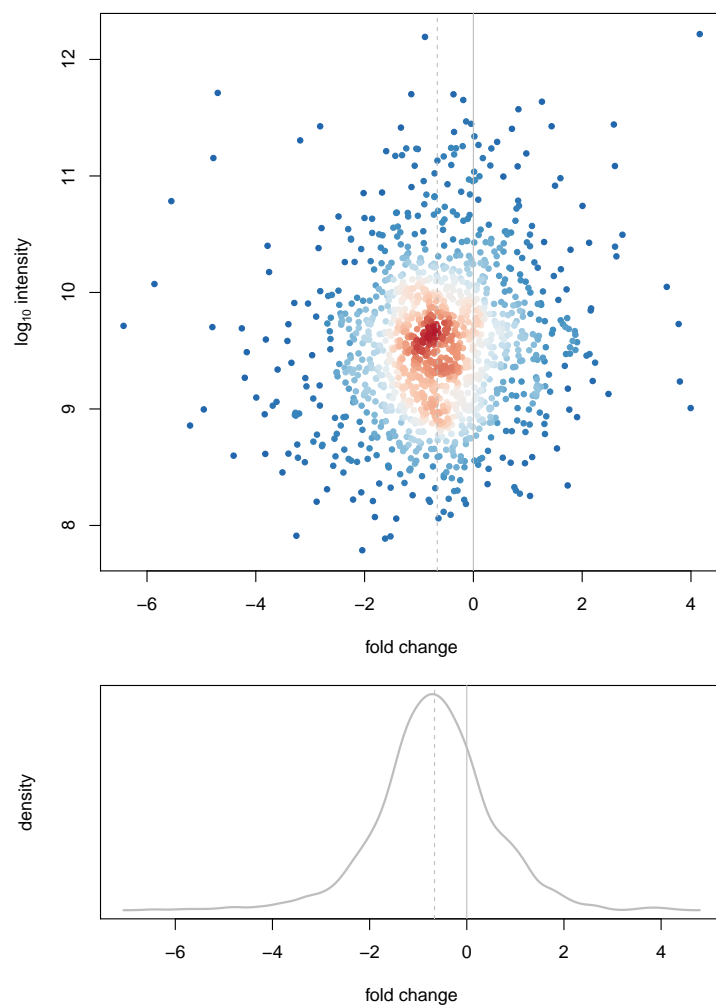median(fc) = −1.3328   sd(fc) = 1.5445

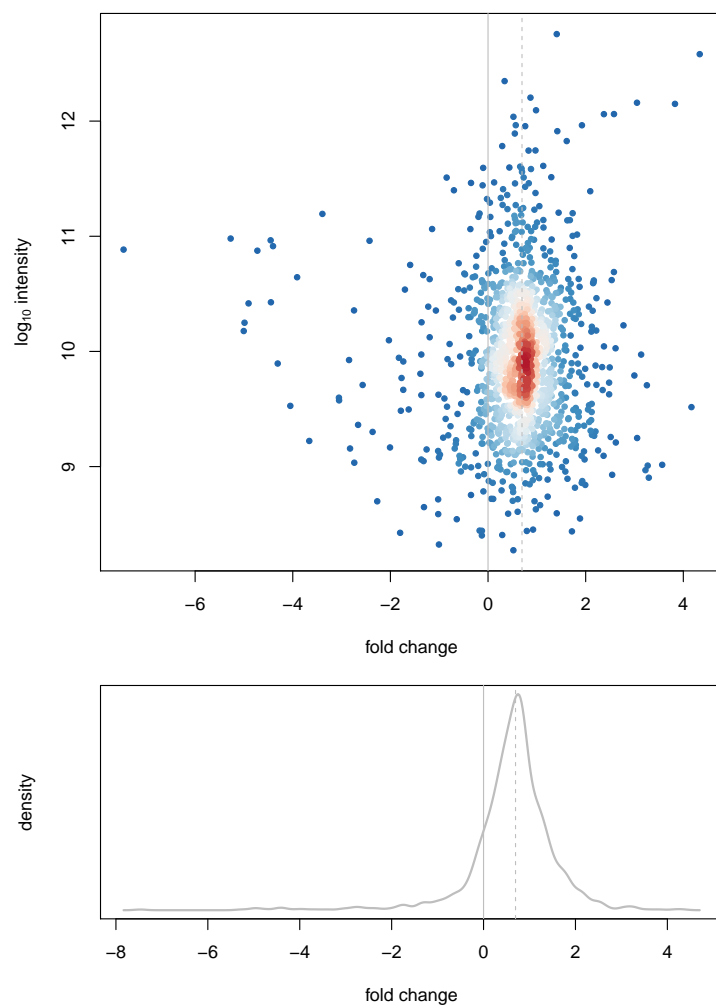Figure 6: Fold changes of peptide abundances 1 and 3.
median(fc) = −0.6641   sd(fc) = 1.1804

Figure 7: Fold changes of peptide abundances 2 and 3.
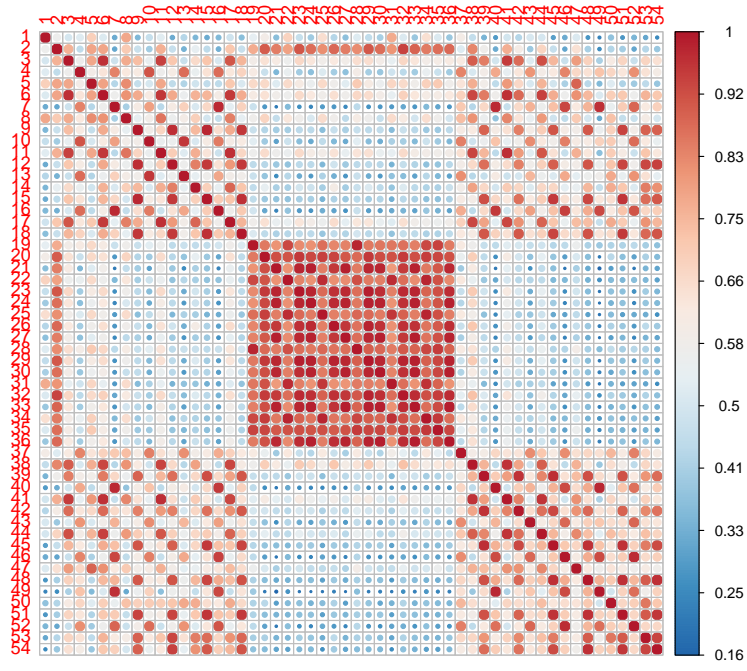median(fc) = 0.6958   sd(fc) = 0.9636
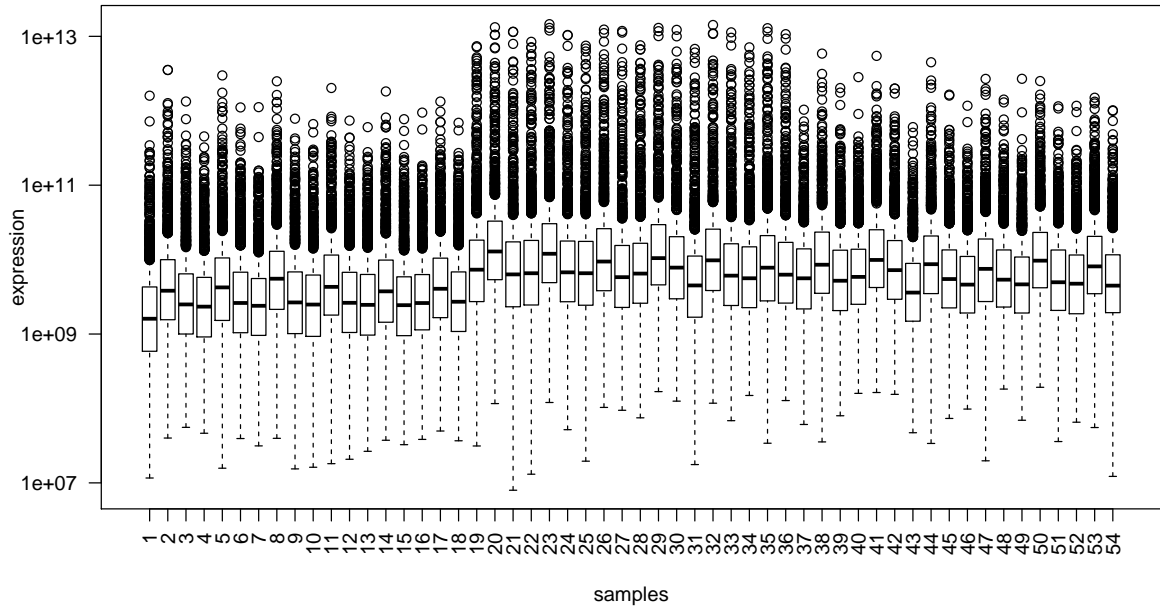
Figure 8: Correlation of all peptide abundances.

Figure 9: Boxplot of all peptide abundances.