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
$\overline{SSAAPPPPPR(Label:13C(6)15N(4))}$	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	\mathbf{C}	150
Label: $13C(6)15N(2)$	K	6
Label: $13C(6)15N(4)$	R	4

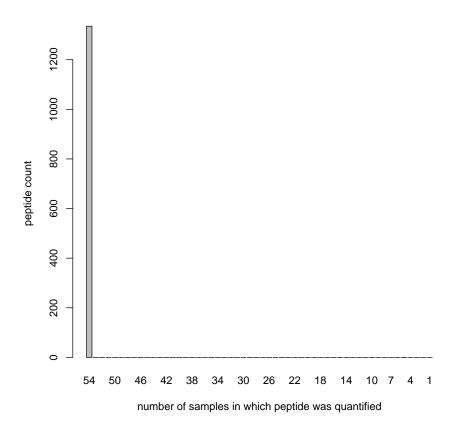
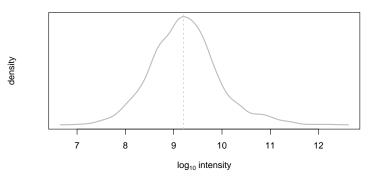
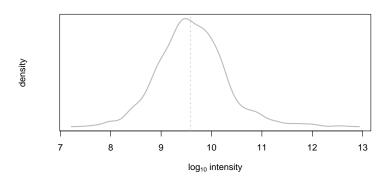


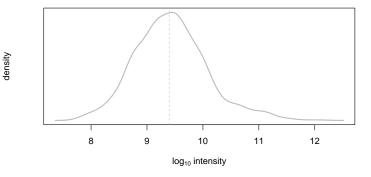
Figure 1: Frequency plot of peptide quantifications.



(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 2: peptide abundance distributions.



Figure 3: Kendrick nominal fractional mass plot

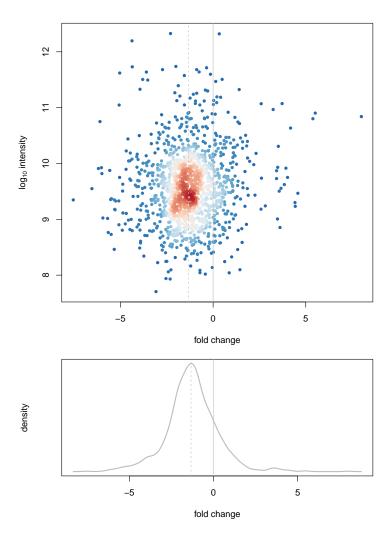


Figure 4: Fold changes of peptide abundances 1 and 2. $\mathrm{median}(\mathrm{fc}) = -1.3328 \qquad \mathrm{sd}(\mathrm{fc}) = 1.5445$

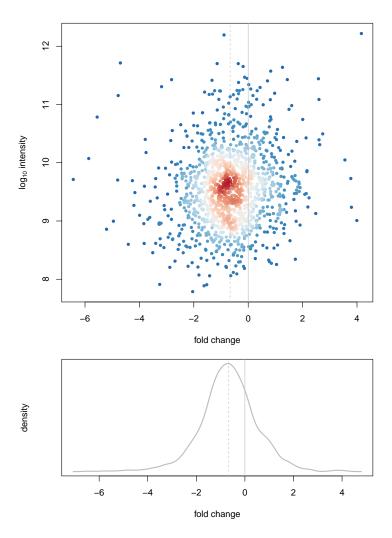


Figure 5: Fold changes of peptide abundances 1 and 3. $median(fc) = -0.6641 \qquad sd(fc) = 1.1804$

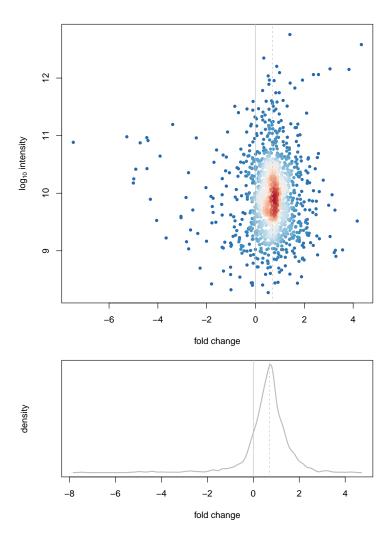


Figure 6: Fold changes of peptide abundances 2 and 3. $median(fc) = 0.6958 \qquad sd(fc) = 0.9636$

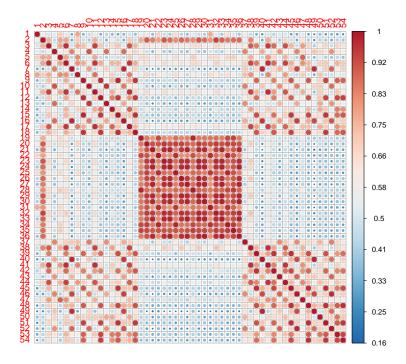


Figure 7: Correlation of all peptide abundances.

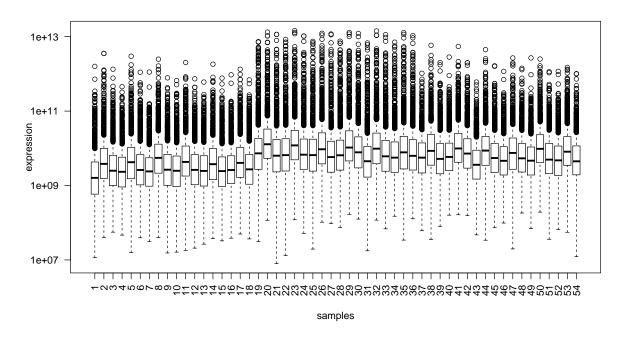


Figure 8: Boxplot of all peptide abundances.