Report for PEP Section in mzTab File
example_5

The PEP section of the mzTab file contains $45,072$ quantified peptide features measured in 54 samples.

	number of peptides
quantified	45,072
identified (total)	45,072
identified (unique modified)	35,080
identified (unique stripped)	31,307

Table 1: Total number of quantified and identified peptides.

modifications statistics

mod	specificity	number
Oxidation	M	8798
Methylthio	C	7927
Dioxidation	M	372
Label:13C(6)15N(4)	R	89
Label:13C(6)15N(2)	K	79

modified sequence	accession	charge	retention time	m/z
SSAAPPPPPR(Label:13C(6)15N(4))	STD_01	2	1659.92	493.77
SSAAPPPPPR(Label:13C(6)15N(4))	STD_01	2	1605.04	493.76
GISNEGQNASIK(Label:13C(6)15N(2))	STD_02	2	2041.39	613.32
GISNEGQNASIK(Label:13C(6)15N(2))	STD_02	1	2043.80	1225.63
HVLTSIGEK(Label:13C(6)15N(2))	STD_03	2	2127.71	496.29
DIPVPK(Label:13C(6)15N(2))PK	STD_04	2	2653.71	451.28
DIPVPKPK(Label:13C(6)15N(2))	STD_04	2	2850.03	451.28
IGDYAGIK(Label:13C(6)15N(2))	STD_05	2	3096.71	422.74
IGDYAGIK(Label:13C(6)15N(2))	STD_05	2	3283.08	422.74
TASEFDSAIAQDK(Label:13C(6)15N(2))	STD_06	2	4266.53	695.83
TASEFDSAIAQDK	STD_06	2	4271.48	691.83
SAAGAFGPELSR(Label:13C(6)15N(4))	STD_07	2	4457.27	586.80
SAAGAFGPELSR(Label:13C(6)15N(4))	STD_07	2	4650.67	586.80
ELGQSGVDTYLQTK(Label:13C(6)15N(2))	STD_08	2	5741.14	773.90
ELGQSGVDTYLQTK(Label:13C(6)15N(2))	STD_08	2	5880.07	773.90
GLILVGGYGTR(Label:13C(6)15N(4))	STD_09	2	6431.53	558.33
GLILVGGYGTR(Label:13C(6)15N(4))	STD_09	2	4427.35	558.33
GILFVGSGVSGGEEGAR	P52209	2	6780.92	796.41
GILFVGSGVSGGEEGAR(Label:13C(6)15N(4))	P52209	2	6781.34	801.41
GILFVGSGVSGGEEGAR(Label:13C(6)15N(4))	P52209	2	6859.38	801.41
SFANQPLEVVYSK(Label:13C(6)15N(2))	STD_11	2	6787.30	745.39
SFANQPLEVVYSK(Label:13C(6)15N(2))	STD_11	2	6606.62	745.39
LTILEELR(Label:13C(6)15N(4))	STD_12	2	7538.66	498.80
LTILEELR(Label:13C(6)15N(4))	STD_12	2	7689.53	498.80
ELASGLSFPVGFK(Label:13C(6)15N(2))	STD_14	2	9083.08	680.37
ELASGLSFPVGFK(Label:13C(6)15N(2))	STD_14	2	8764.02	680.37
LSSEAPALFQFDLK(Label:13C(6)15N(2))	STD_15	2	9657.05	787.42
AKGILFVGSGVSGGEEGAR	P52209	3	4941.74	597.65

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
DLQVKPGESLEVIQTTDDTK	O15117	3	6929.06	739.38
FGTPASLTTR	O15117	2	3832.43	525.79
FGTPASLTTRDPEAK	O15117	3	3573.64	530.94
FGTPASLTTRDPEAK	O15117	2	3552.42	795.91
GQTSYSTTSLPPPPPSHPASQPPLPASHPSQPPVPSLPPR	O15117	4	6523.22	1023.03
GSPAPLGVR	O15117	2	2591.06	427.25
INQEELASGTPPARFPK	O15117	3	4675.29	618.99
KNLFNNQGNASPPAGPSNVPK	O15117	3	3789.84	717.70
LTGPIQVIHLAK	O15117	3	5722.29	430.60
NLFNNQGNASPPAGPSNVPK	O15117	2	5245.34	1012.00
QGEQIEIIR	O15117	2	4463.55	543.30
SGPTPPTSENEQK	O15117	2	1578.46	686.32
SGPTPPTSENEQKQAFPK	O15117	3	2664.43	648.32
SGPTPPTSENEQKQAFPK	O15117	2	2665.14	971.98
TTAVEIDYDSLK	O15117	2	6256.92	677.84
VGFLKPVGPKPINLPK	O15117	3	5331.98	568.69
VTGPNSSSGIQAR	O15117	2	1967.01	637.33
YNTGGNPTEDVSVNSRPFR	O15117	3	4621.45	704.00

Table 3: Proteins of interest.
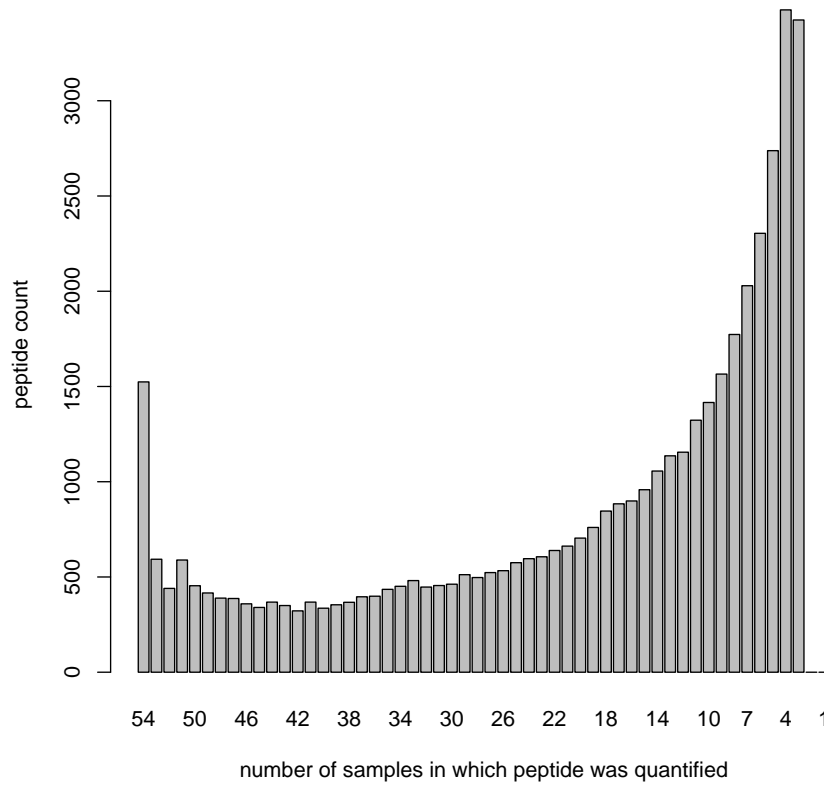
Figure 1: Frequency plot of peptide quantifications.
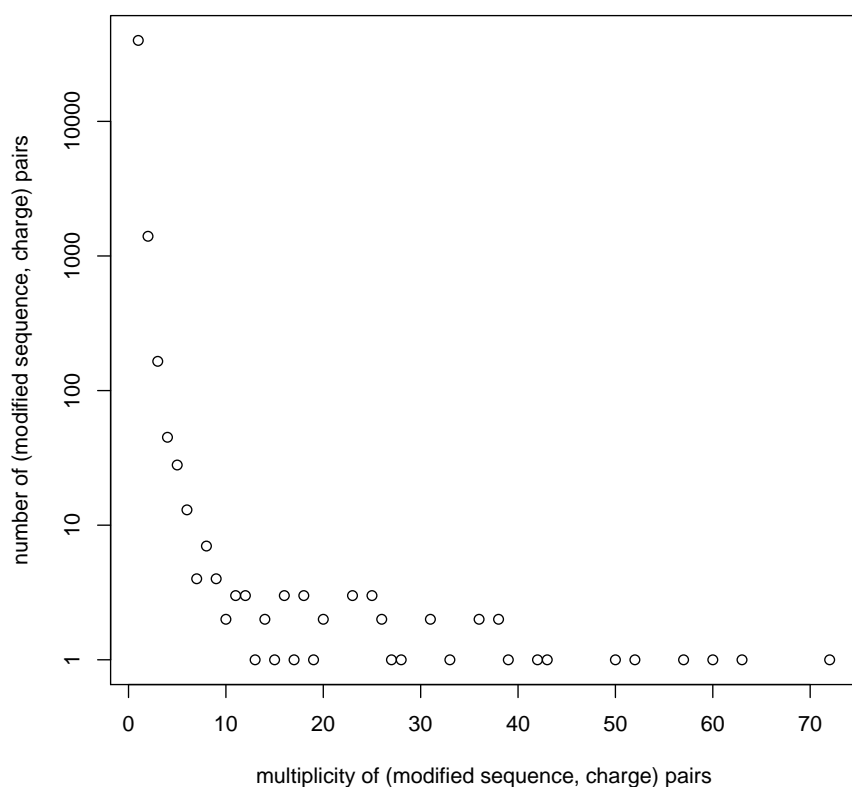
Figure 2: (modified sequence, charge) pair multiplicity vs frequency plot. Each peptide feature (characterised by a (possibly) modified peptide sequence and a charge state) should ideally occur only once in the analysis. In other words, peptides of multiplicity 1 should have a very high frequency. The plot below should show a significant spike on the left and can be used as QC of the analysis.
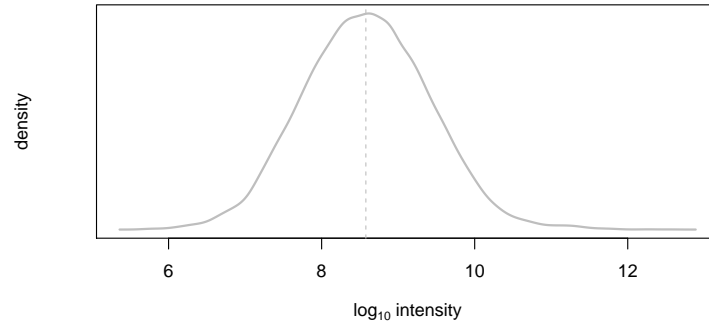
(a) peptide abundances 1, median(intensity) = 378, 509, 488
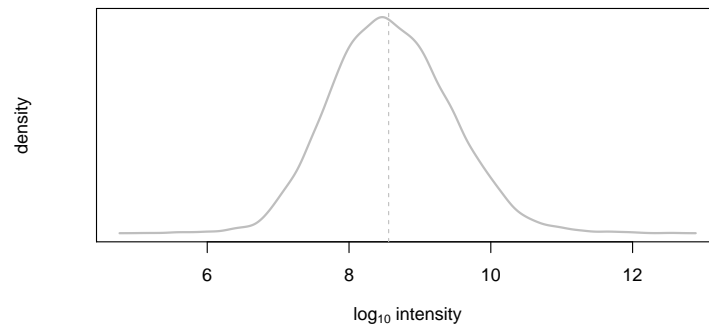
(b) peptide abundances 2, median(intensity) = 362, 260, 000
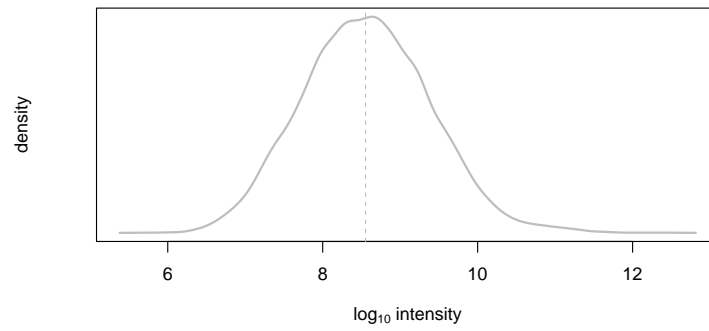
(c) peptide abundances 3, median(intensity) = 357, 520, 000

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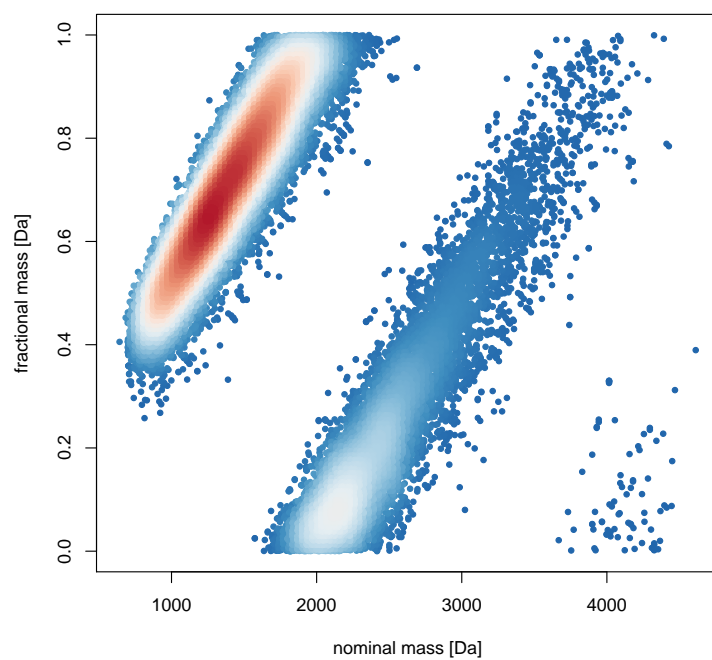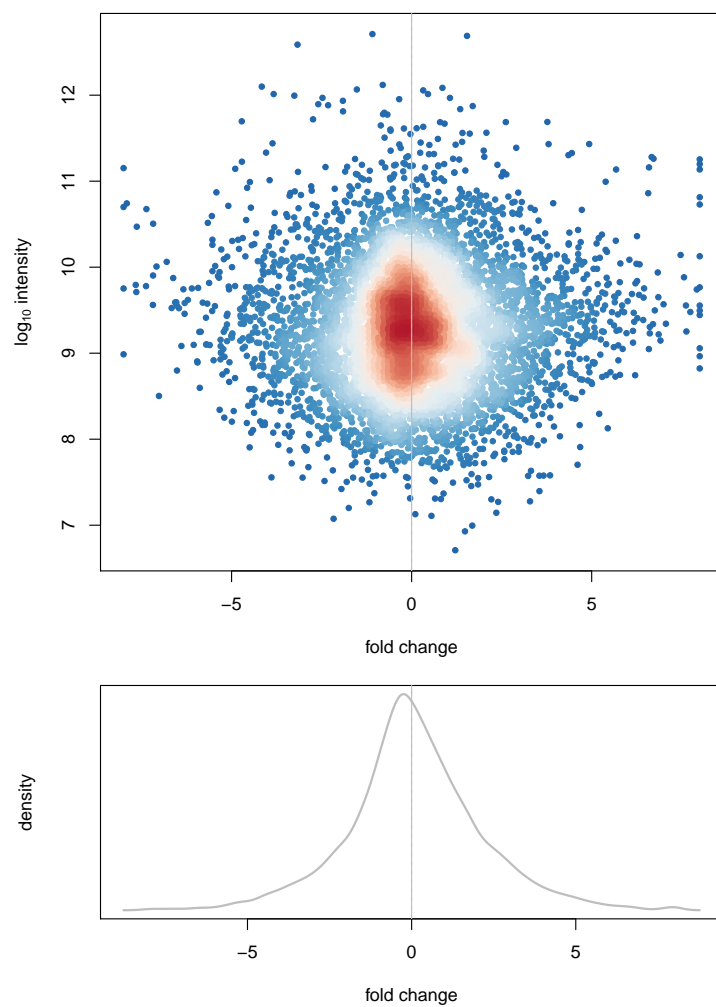
Figure 4: Kendrick nominal fractional mass plot

Figure 5: Fold changes of peptide abundances 1 and 2.
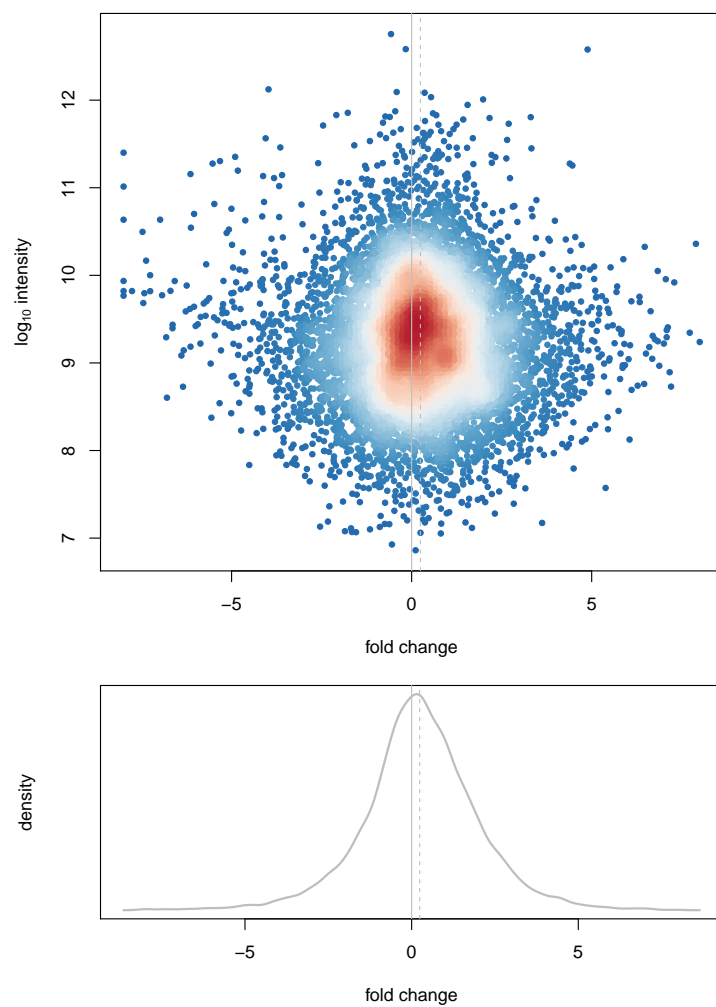median(fc) = −0.0034   sd(fc) = 2.0759

Figure 6: Fold changes of peptide abundances 1 and 3.
median(fc) = 0.2428   sd(fc) = 1.7662

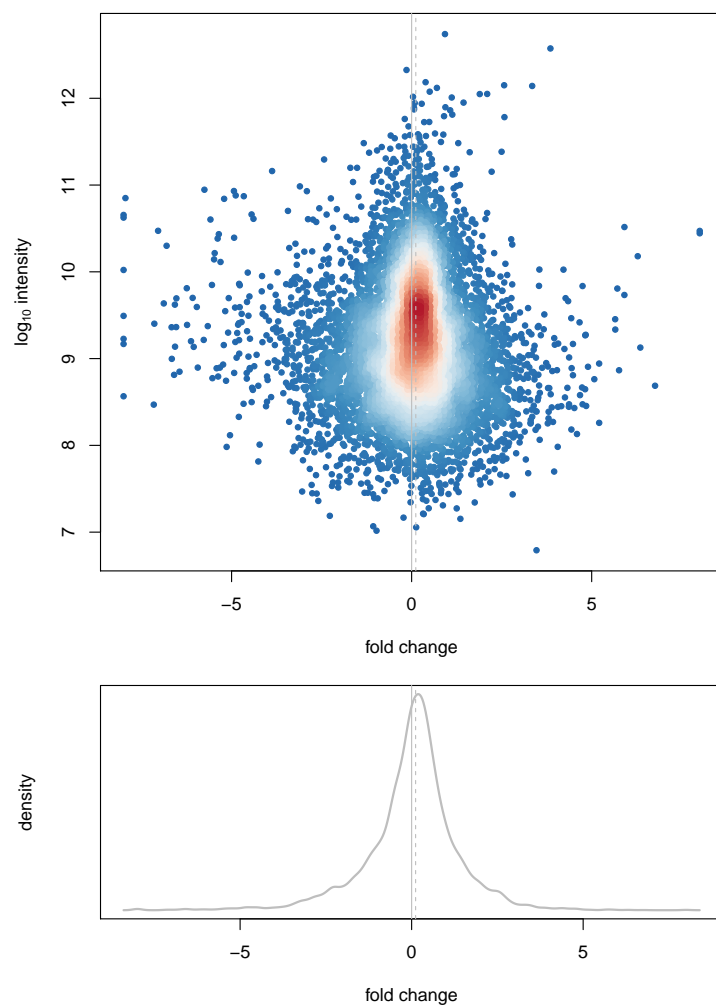Figure 7: Fold changes of peptide abundances 2 and 3.
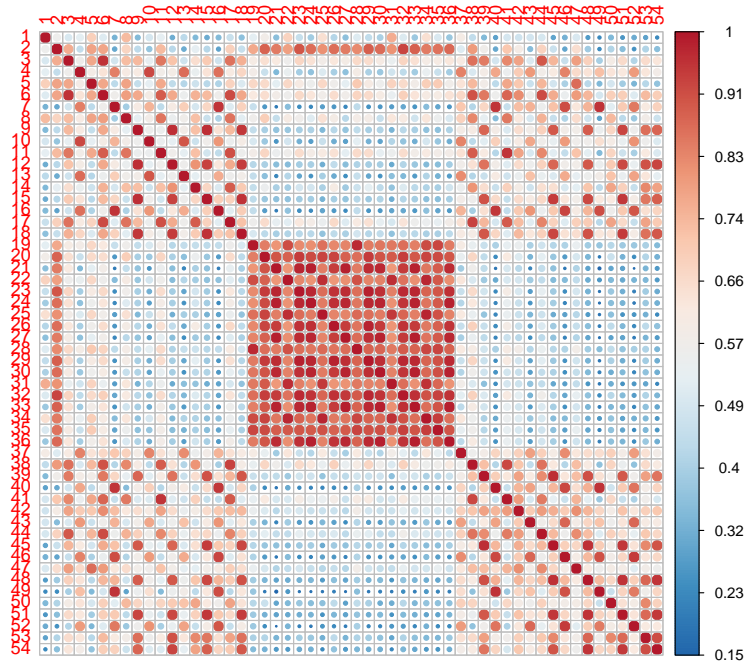median(fc) = 0.1159   sd(fc) = 1.3579
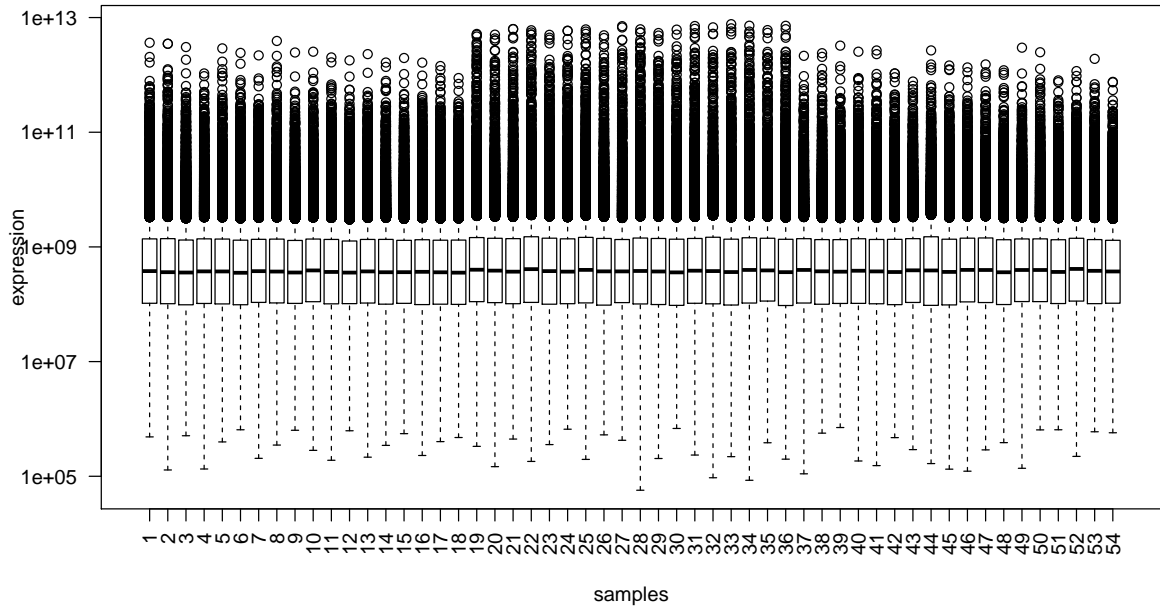
Figure 8: Correlation of all peptide abundances.

Figure 9: Boxplot of all peptide abundances.