Report for `PEP` Section in `mzTab` File
example_2

The `PEP` section of the `mzTab` file contains $2,160$ quantified peptide features measured in 2 samples.

	number of peptides
quantified	2,160
identified (total)	2,160
identified (unique modified)	2,021
identified (unique stripped)	1,926

Table 1: Total number of quantified and identified peptides.

modified sequence	accession	charge	retention time	m/z
no matching sequences found				

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
(Dimethyl)ATYTQTHMDFIIEAFK(Dimethyl)
(Dimethyl:2H(4)13C(2))ATYTQTHMDFIIEAFK(Dimethyl:2H(4)13C(2))
(Dimethyl)ATYTQTHMDFIIEAFK(Dimethyl)
(Dimethyl)ATYTQTHMDFIIEAFK(Dimethyl)
(Dimethyl)ATYTQTHMDFIIEAFK(Dimethyl)
(Dimethyl)AVEIGSFLLGR
(Dimethyl:2H(4)13C(2))AVEIGSFLLGR
(Dimethyl)DAMVPMGGLLC(Carbamidomethyl)MK(Dimethyl)
(Dimethyl)DAMVPMGGLLC(Carbamidomethyl)MK(Dimethyl)
(Dimethyl:2H(4)13C(2))DDSFFDVYTEC(Carbamidomethyl)R
(Dimethyl:2H(4)13C(2))DDSFFDVYTEC(Carbamidomethyl)R
(Dimethyl)DWTIEQITR
(Dimethyl)EAEYK(Dimethyl)DWTIEQITR
(Dimethyl)EAEYK(Dimethyl)DWTIEQITR
(Dimethyl)EAFDTGVR
(Dimethyl:2H(4)13C(2))FAENAYFIK(Dimethyl:2H(4)13C(2))
(Dimethyl)GAEQIYIPVLIK(Dimethyl)
(Dimethyl)GAEQIYIPVLIK(Dimethyl)
(Dimethyl)GAEQIYIPVLIK(Dimethyl)K(Dimethyl)
(Dimethyl:2H(4)13C(2))GDEAYSGSR
(Dimethyl:2H(4)13C(2))GIEEVGPNNVPYIVATITSNSAGGQPVSLANLK(Dimethyl:2H(4)13C(2))
(Dimethyl:2H(4)13C(2))GIEEVGPNNVPYIVATITSNSAGGQPVSLANLK(Dimethyl:2H(4)13C(2))
(Dimethyl)GIEEVGPNNVPYIVATITSNSAGGQPVSLANLK(Dimethyl)
(Dimethyl:2H(4)13C(2))GLTFTYEPK(Dimethyl:2H(4)13C(2))
(Dimethyl)GNFDLEGLER
(Dimethyl)HLPEPFR
(Dimethyl)HLPEPFR
(Dimethyl:2H(4)13C(2))HLPEPFR
(Dimethyl)IAQVQYLVDGLEEIGVVC(Carbamidomethyl)QQAGGHAAFVDAGK(Dimethyl)
(Dimethyl:2H(4)13C(2))K(Dimethyl:2H(4)13C(2))DAMVPMGGLLC(Carbamidomethyl)MK(Dimethyl:2H(4)13C(2))
(Dimethyl:2H(4)13C(2))K(Dimethyl:2H(4)13C(2))YDIPVVMDSAR
(Dimethyl)K(Dimethyl)YDIPVVMDSAR
(Dimethyl)LAVGLYDGMNLDWLAYR
(Dimethyl)LAVGLYDGMNLDWLAYR
(Dimethyl:2H(4)13C(2))LLPHIPADQFPAQALAC(Carbamidomethyl)ELYK(Dimethyl:2H(4)13C(2))
(Dimethyl:2H(4)13C(2))LLPHIPADQFPAQALAC(Carbamidomethyl)ELYK(Dimethyl:2H(4)13C(2))
(Dimethyl:2H(4)13C(2))LLPHIPADQFPAQALAC(Carbamidomethyl)ELYK(Dimethyl:2H(4)13C(2))
(Dimethyl)LLPHIPADQFPAQALAC(Carbamidomethyl)ELYK(Dimethyl)
(Dimethyl:2H(4)13C(2))NIFGYQYTIPTHQGR
(Dimethyl:2H(4)13C(2))NIFGYQYTIPTHQGR
(Dimethyl:2H(4)13C(2))QLPC(Carbamidomethyl)PAELLR
(Dimethyl)SYYALAESVK(Dimethyl)
(Dimethyl:2H(4)13C(2))TLC(Carbamidomethyl)VVQEGFPTYGGLEGGAMER
(Dimethyl)TLC(Carbamidomethyl)VVQEGFPTYGGLEGGAMER
(Dimethyl:2H(4)13C(2))GADSC(Carbamidomethyl)LVSIAGEGLVDVPAVK(Dimethyl:2H(4)13C(2))
(Dimethyl)GFGGDTLNTSVYIAR
(Dimethyl:2H(4)13C(2))GHLTASTVIQYR
(Dimethyl)IAVIGEC(Carbamidomethyl)MIELSEK(Dimethyl)
(Dimethyl)LPGLYYIETDSTGER
(Dimethyl:2H(4)13C(2))LPGLYYIETDSTGER
(Dimethyl:2H(4)13C(2))VIDTTAAGDSFSAGYLAVR

Table 3: Proteins of interest.

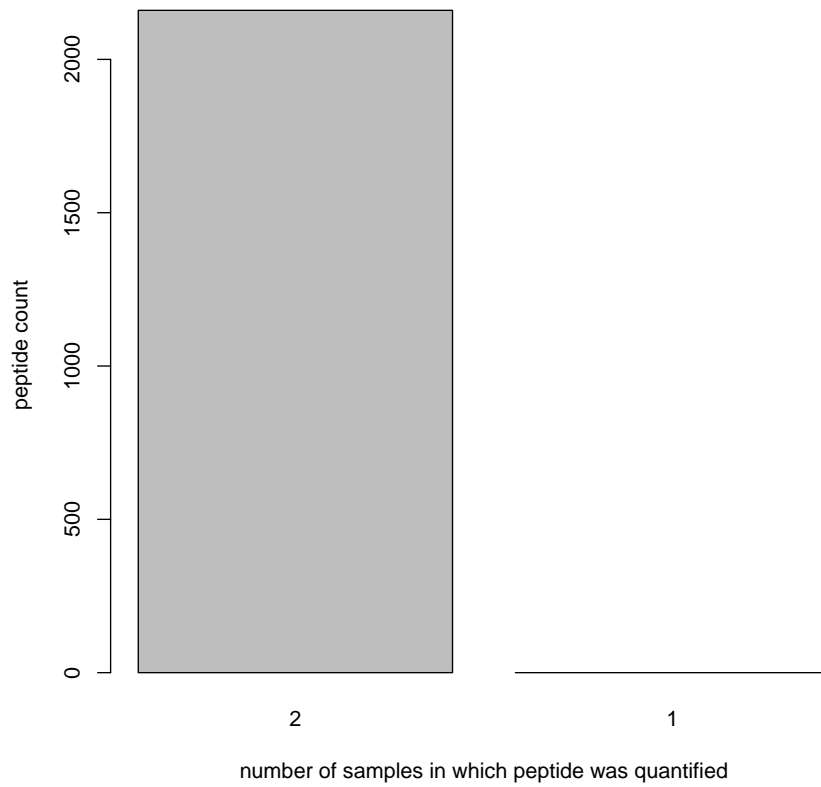| mod	specificity	number
Carbamidomethyl	C	205

Table 4: Statistics of modifications.

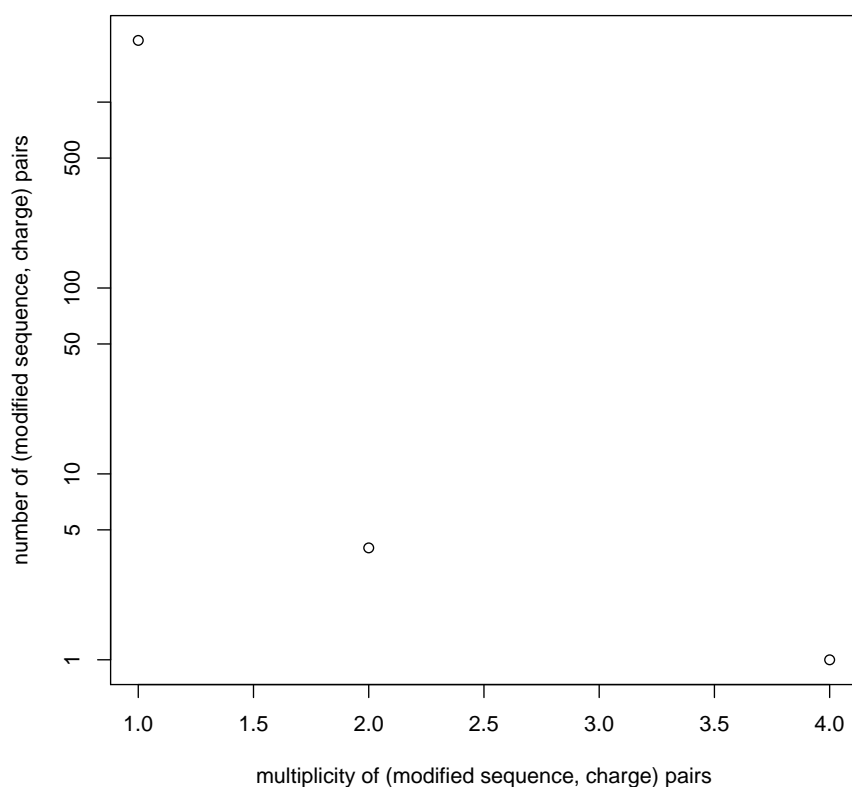Figure 1: Frequency plot of peptide quantifications.

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.
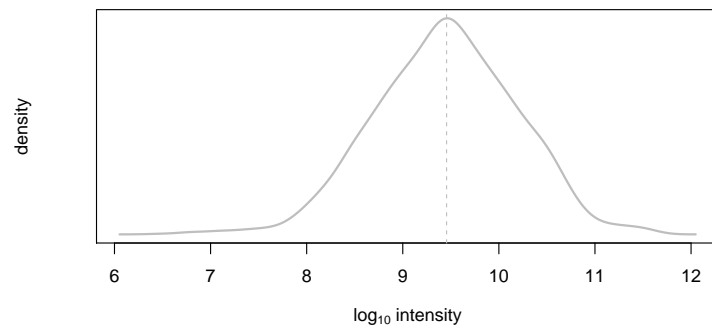
(a) peptide abundances 1, median(intensity) = 2, 858, 004, 992
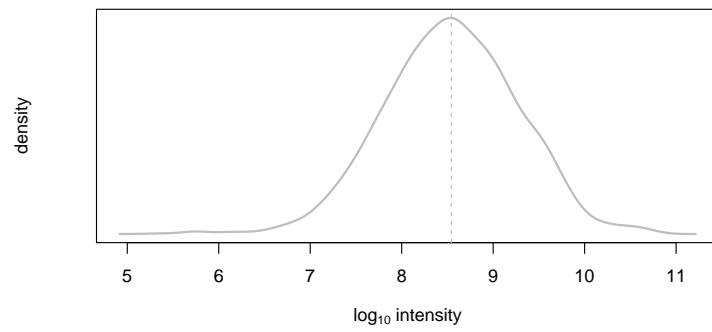
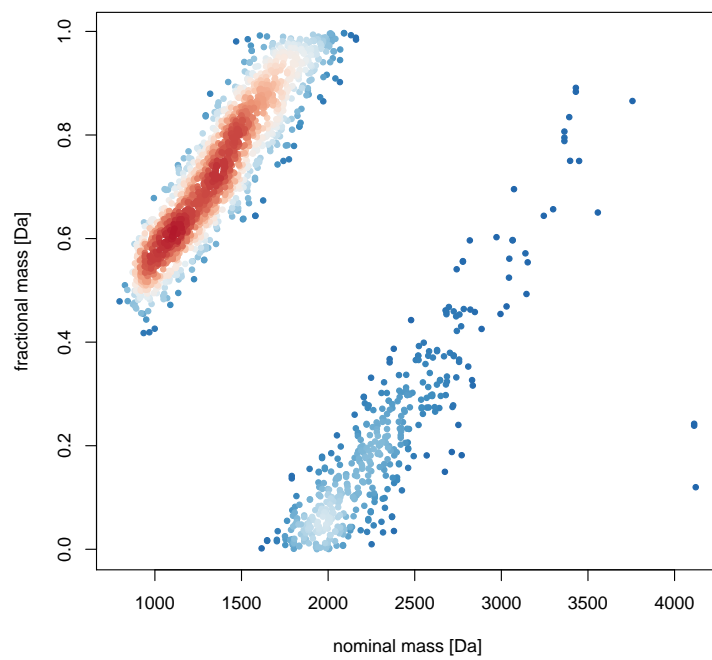(b) peptide abundances 2, median(intensity) = 348, 081, 008

Figure 3: peptide abundance distributions.

Figure 4: Kendrick nominal fractional mass plot

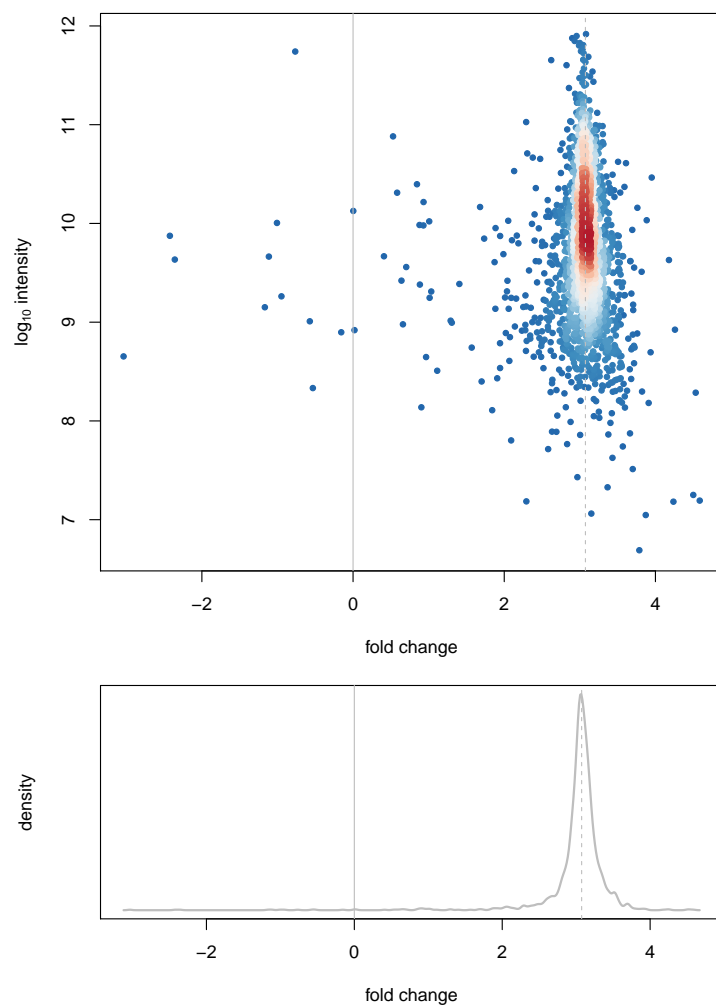Figure 5: Fold changes of peptide abundances 1 and 2.
median(fc) = 3.0739   sd(fc) = 0.4645