

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.

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

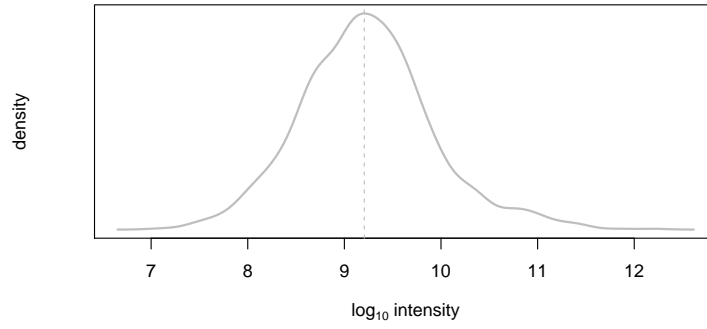
Table 2: Statistics of modifications.



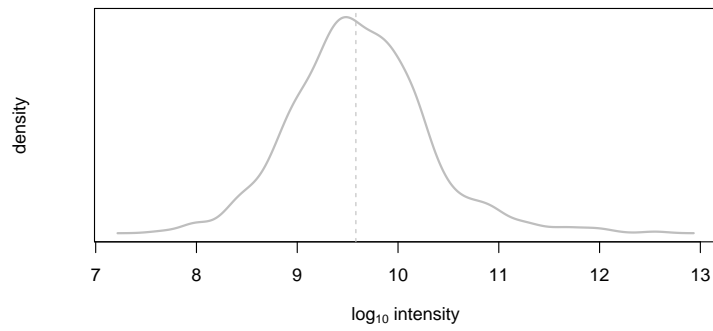
Figure 1: Frequency plot of peptide quantifications.



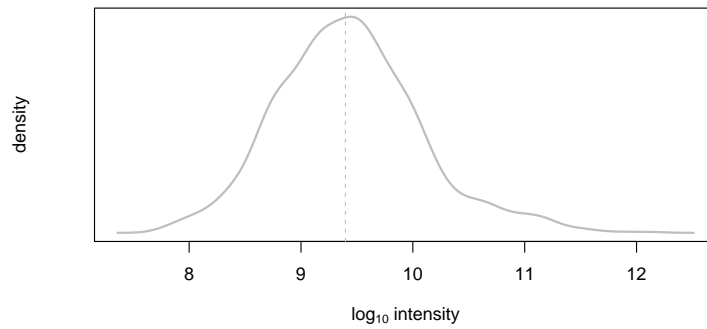
Figure 2: (modified sequence, charge) pair multiplicity vs frequency plot. Each peptide feature (characterised by a (possibly) modified peptide sequence and a charge state) should ideally occur only once in the analysis. In other words, peptides of multiplicity 1 should have a very high frequency. The plot below should show a significant spike on the left and can be used as QC of the analysis.



(a) peptide abundances 1, $\text{median}(\text{intensity}) = 1,605,469,952$



(b) peptide abundances 2, $\text{median}(\text{intensity}) = 3,819,539,968$



(c) peptide abundances 3, $\text{median}(\text{intensity}) = 2,497,959,936$

Figure 3: peptide abundance distributions.

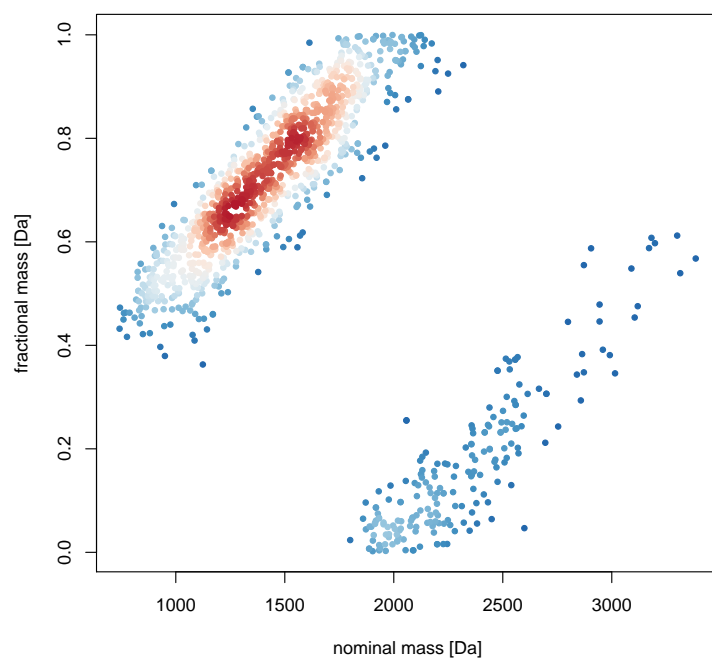


Figure 4: Kendrick nominal fractional mass plot

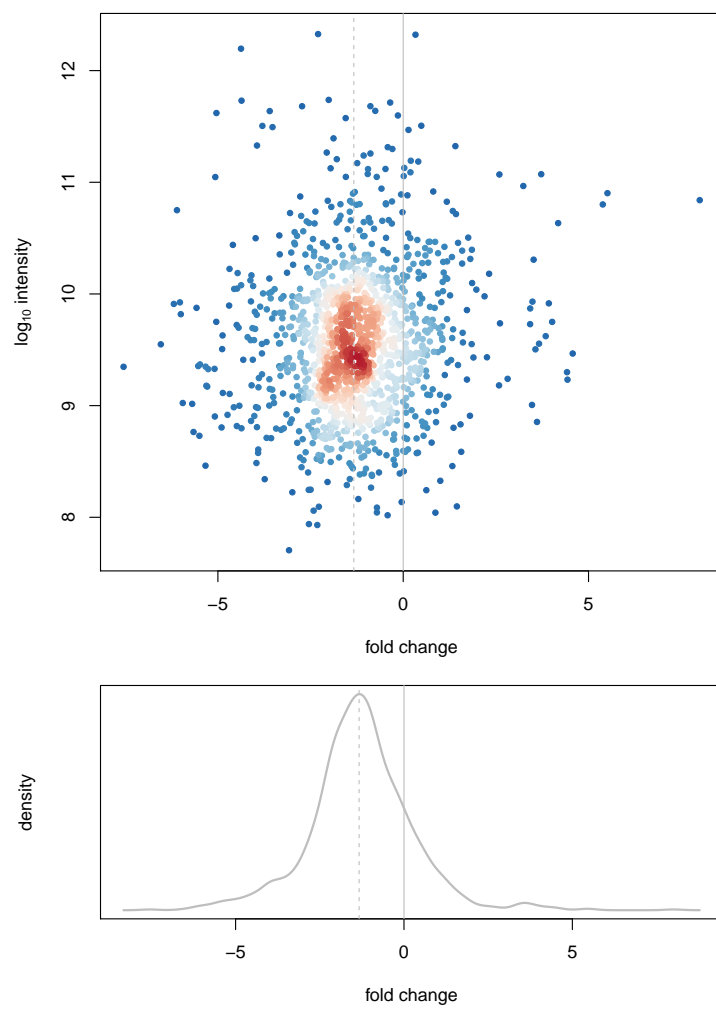


Figure 5: Fold changes of peptide abundances 1 and 2.
 $\text{median}(\text{fc}) = -1.3328$ $\text{sd}(\text{fc}) = 1.5445$

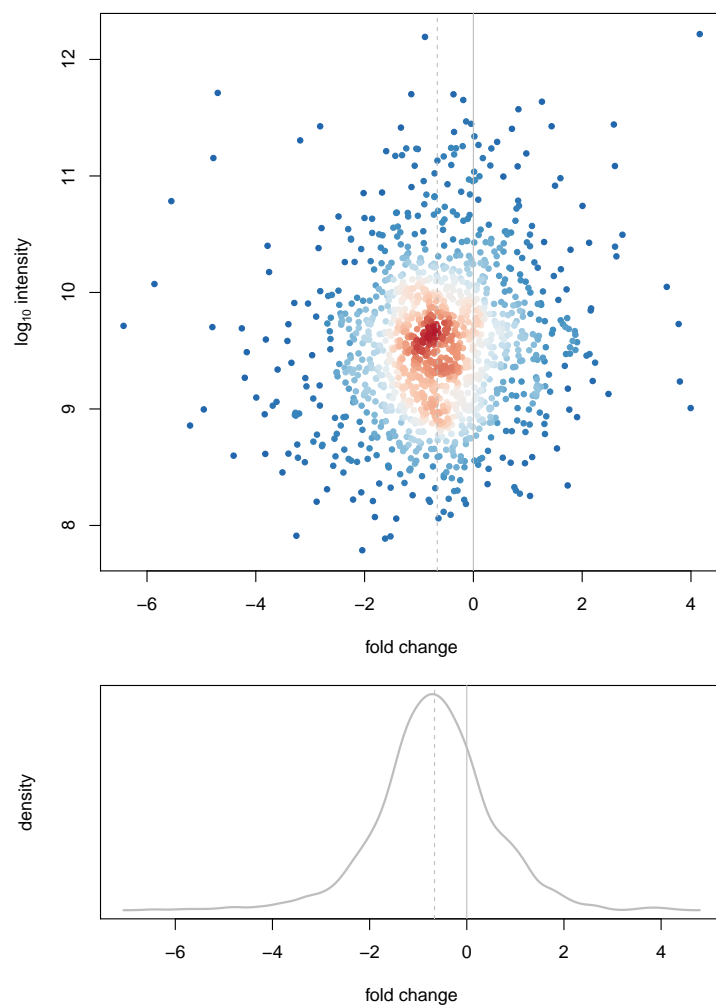


Figure 6: Fold changes of peptide abundances 1 and 3.
 $\text{median}(\text{fc}) = -0.6641$ $\text{sd}(\text{fc}) = 1.1804$

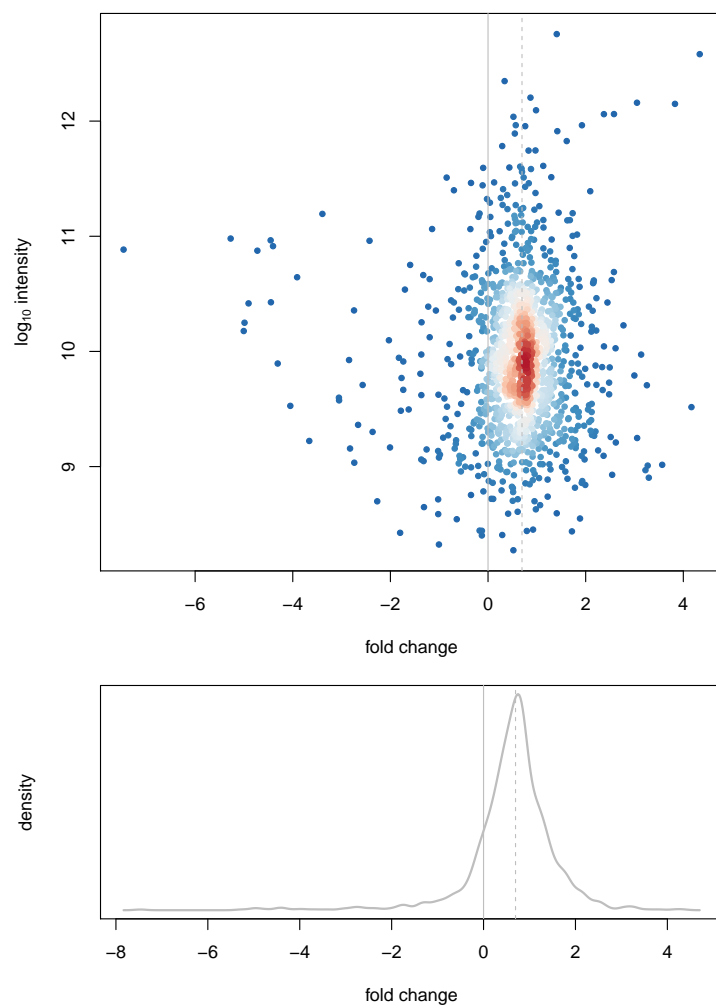


Figure 7: Fold changes of peptide abundances 2 and 3.
 $\text{median}(\text{fc}) = 0.6958$ $\text{sd}(\text{fc}) = 0.9636$

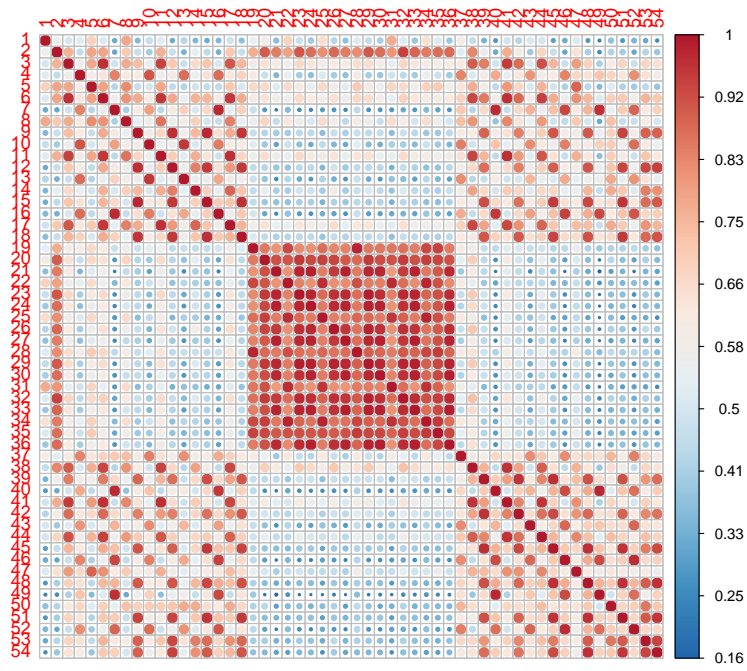


Figure 8: Pearson correlation of all peptide abundances. (min correlation = 0.1622, median correlation = 0.5936, max correlation = 1)

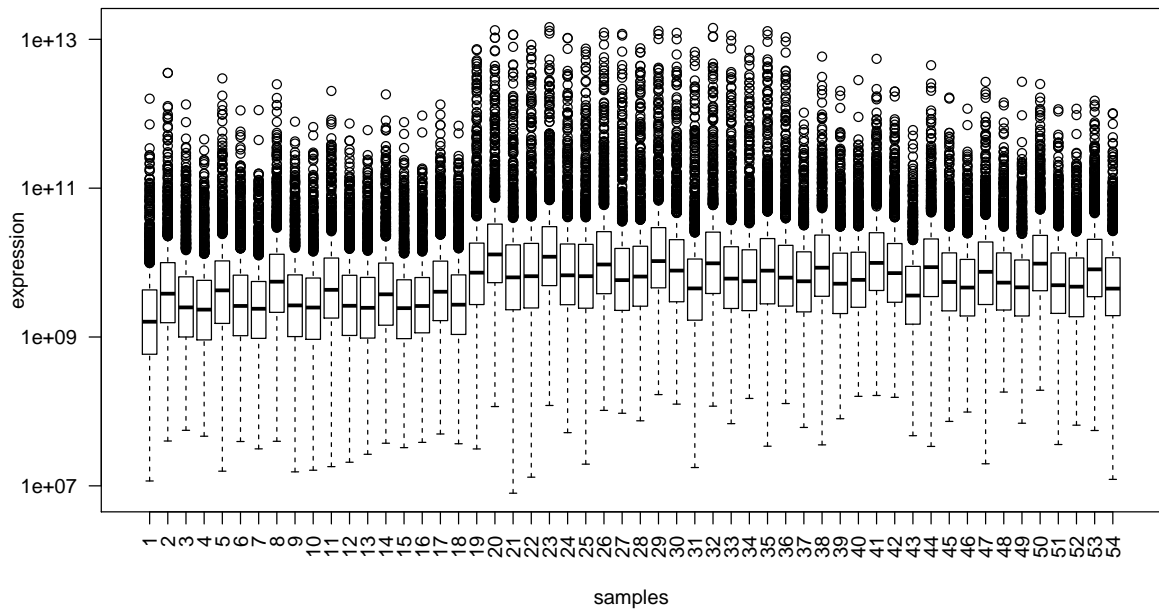


Figure 9: Boxplot of all peptide abundances.

| modified sequence | accession | charge | retention time | m/z |
|-------------------------|-----------|--------|----------------|--------|
| GNFGGSFAGSFGGAGGHAPGVAR | P52272 | 3 | 5570.46 | 678.99 |

Table 3: 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.

| modified sequence | accession | charge | retention time | m/z |
|------------------------------|-----------|--------|----------------|---------|
| AHGGYSVFAGVGER | P06576 | 3 | 4066.84 | 469.57 |
| FLSQPFQVAEVFTGHM(Oxidatio... | P06576 | 3 | 8779.41 | 680.34 |
| FTQAGSEVSALLGR | P06576 | 2 | 7458.45 | 718.38 |
| IM(Oxidation)DPNIVGSEHYDV... | P06576 | 3 | 4749.42 | 611.29 |
| IM(Oxidation)NVIGEPIDERGP... | P06576 | 3 | 5343.69 | 599.66 |
| LVLEVAQHLGESTVR | P06576 | 3 | 6607.33 | 550.98 |
| TIAM(Oxidation)DGTEGLVR | P06576 | 2 | 4113.14 | 639.82 |
| VALVYGQM(Oxidation)NEPPGA... | P06576 | 2 | 4560.45 | 809.41 |
| VLDSGAPIKIPVGPETLGR | P06576 | 3 | 7703.51 | 640.37 |
| VLDSGAPIKIPVGPETLGR | P06576 | 2 | 7703.86 | 960.05 |
| VVDLLAPYAK | P06576 | 2 | 7025.47 | 544.82 |
| GFAFVQYVNER | P07910 | 2 | 7451.91 | 665.33 |
| M(Oxidation)IAGQVLDINLAAE... | P07910 | 2 | 8127.15 | 849.96 |
| MIAGQVLDINLAAEPK | P07910 | 2 | 8833.20 | 841.96 |
| VPPPPPIAR | P07910 | 2 | 3073.40 | 472.29 |
| AGTQIENIDEDFRDGLK | O43707 | 3 | 6848.07 | 640.98 |
| AIM(Oxidation)TYVSSFYHAFS... | O43707 | 3 | 8185.78 | 675.32 |
| ALDFIASK | O43707 | 2 | 4963.37 | 432.74 |
| DGLAFNALIHR | O43707 | 2 | 7035.73 | 613.84 |
| ELPPDQAEYC(Methylthio)IAR | O43707 | 2 | 6999.29 | 775.85 |
| ETTDTDADQVIASFK | O43707 | 2 | 8062.69 | 871.41 |
| LSGSNPYTTVTPQIINSK | O43707 | 2 | 6625.51 | 960.51 |
| LVSIGAEIIVDGNK | O43707 | 2 | 6663.17 | 757.91 |
| M(Oxidation)APYQGPDAVPGAL... | O43707 | 2 | 6433.07 | 904.93 |
| M(Oxidation)LDAEDIVNTARPD... | O43707 | 3 | 5738.10 | 611.63 |
| M(Oxidation)LDAEDIVNTARPD... | O43707 | 2 | 5737.40 | 916.94 |
| TINEVENQILTR | O43707 | 2 | 6198.35 | 715.39 |
| DNHLLGTFDLTGIPPAPR | P11021 | 3 | 9502.66 | 645.34 |
| IDTRNELESYAYSLK | P11021 | 3 | 6935.43 | 601.30 |
| IINEPTAAAIAAYGLDK | P11021 | 2 | 8020.47 | 830.45 |
| ITPSYVAFTPEGER | P11021 | 2 | 6421.94 | 783.89 |
| LYGSAGPPPTGEEDTAEKDEL | P11021 | 2 | 5768.97 | 1088.50 |
| NQLTSNPENTVFDAK | P11021 | 2 | 5446.82 | 839.41 |
| NQLTSNPENTVFDAKR | P11021 | 3 | 4260.53 | 611.97 |
| SQIFSTASDNQPTVTIK | P11021 | 2 | 6081.44 | 918.97 |
| TKPYIQVDIGGGQTK | P11021 | 3 | 4136.75 | 535.63 |
| TWNDPSVQQDIK | P11021 | 2 | 4695.89 | 715.85 |
| VTHAVVTVPAYFNDAQR | P11021 | 3 | 5758.44 | 629.99 |
| VYGERPLTK | P11021 | 2 | 1926.05 | 596.32 |
| IYVDDGLISLQVK | P14618 | 2 | 8923.18 | 731.91 |
| KGVNLPGAAVDLPAVSEKDIQDLK | P14618 | 4 | 7868.62 | 620.10 |
| KGVNLPGAAVDLPAVSEKDIQDLK | P14618 | 3 | 7867.84 | 826.46 |
| SVETLKEM(Oxidation)IK | P14618 | 2 | 2674.97 | 597.33 |
| LIDFLEC(Methylthio)GK | P17844 | 2 | 9345.30 | 542.26 |
| IASLEVENQSLR | P29692 | 2 | 5007.93 | 679.87 |
| SLAGSSGPGASSGTSGDHGELVVR | P29692 | 3 | 3552.50 | 729.02 |
| EATNPPVIQEEKPK | P30101 | 3 | 2402.50 | 527.28 |

| | | | | |
|------------------------------|--------|---|---------|--------|
| FLQDYFDGNLKR | P30101 | 3 | 6540.39 | 505.92 |
| FVM(Oxidation)QEEFSR | P30101 | 2 | 3414.10 | 594.77 |
| GFPTIYFSPANK | P30101 | 2 | 7787.46 | 671.35 |
| GFPTIYFSPANKK | P30101 | 2 | 5901.08 | 735.39 |
| GFPTIYFSPANKK | P30101 | 3 | 5900.67 | 490.60 |
| IFRDGEEAGAYDGPR | P30101 | 2 | 3383.93 | 826.89 |
| IFRDGEEAGAYDGPR | P30101 | 3 | 3384.40 | 551.59 |
| LKGIVPLAK | P30101 | 2 | 3181.18 | 469.82 |
| LSKDPNIVIAK | P30101 | 2 | 2868.45 | 599.36 |
| M(Oxidation)DATANDVPSPYEV... | P30101 | 2 | 5066.94 | 840.88 |
| YGVSGYPTLK | P30101 | 2 | 4804.40 | 542.79 |
| AGGIETIANEYSDR | P34932 | 2 | 5849.11 | 748.35 |
| AIADTGANVVVTGCK | P50990 | 2 | 4341.17 | 686.87 |
| HFSGLEEAVYR | P50990 | 2 | 4456.90 | 654.32 |
| LVPGGGATEIELAK | P50990 | 2 | 5643.63 | 677.88 |
| NLRDIDEVSSLLR | P50990 | 3 | 7752.87 | 510.61 |

Table 4: Proteins of interest.