MS-DAP: Mass Spectrometry Downstream Analysis Pipeline

version: beta 0.2.1   https://github.com/ftwkoopmans/msdap/

Contents

1 Quality control

The quality control figures in this section enable you to investigate reproducibility and global clustering of samples by visualizing:

- number of peptides/proteins detected in each sample
- dataset completeness
- local effects in HPLC peptide retention time per sample
- reproducibility of peptide quantification among replicates
- PCA of all samples to visualize clustering

The first set of quality control figures describes individual samples, thereafter group-level quality metrics are described and finally sample clustering is used to highlight structure in the entire dataset.

1.1 number of peptides and proteins

These plots show the number of (target) peptides that are 'detected' per sample. For DDA, 'detected' implies the peptide has a MS/MS identification. Peptides quantified through match-between-runs (MBR) are quantified but not detected/identified. In case of DDA, we also show the number of peptides quantified through MBR. For DIA, we refer to a peptide as 'detected' if the confidence score (for identification) is $<= 0.01$.

Samples in this plot are sorted by their experimental group, and then ordered and by their name within each group. This data is also available in the output table 'samples.xlsx'.
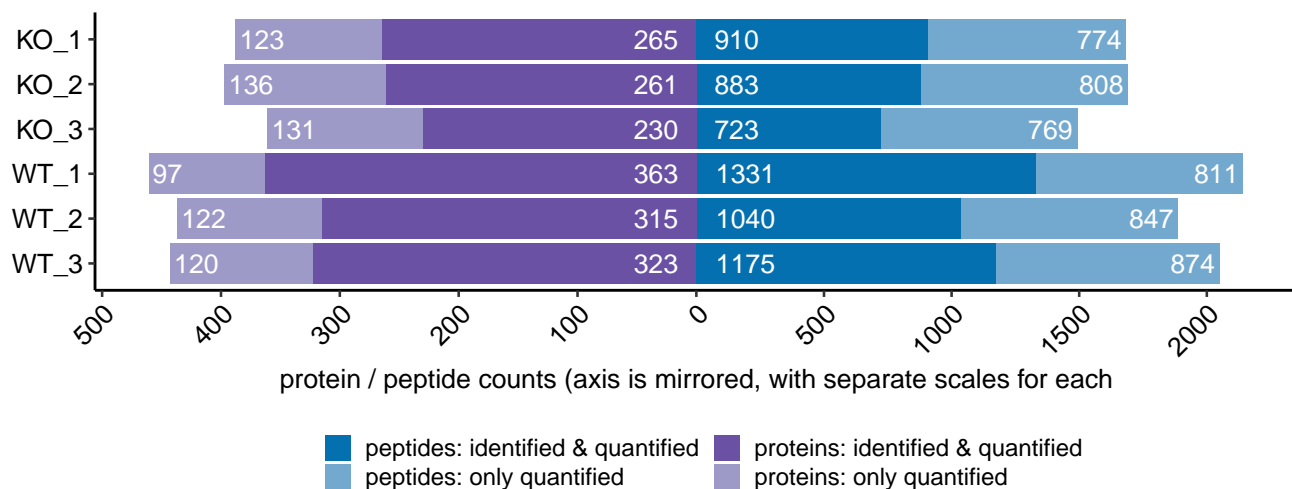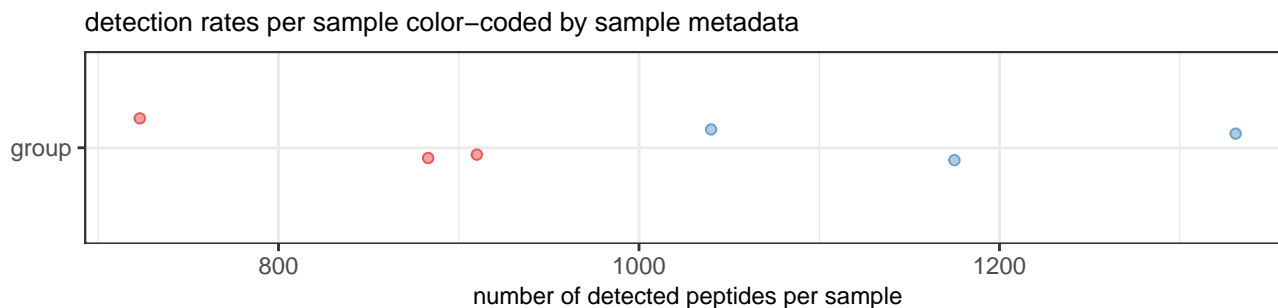
1.1.1 color-coding sample metadata

The number of detected peptides in a sample, as compared to other samples within a dataset, can be used as a measure for sample quality. Color-coding individual samples for metadata that you provided as input (e.g. experiment batch, sample handling order, gel lanes, etc.) allows visual inspection as to whether these relate to the rate of successful peptide detection.

The figure below aims to provide an overview of all sample metadata at a first glance. The y-axis shows all sample metadata. On each row all samples in the dataset are shown as a dot, each color-coded by the respective property shown on the y-axis (with minor vertical jitter for visual clarity). If there is a major effect of any experimental condition on the number of detected peptides, this is easily spotted as all outlier samples (extremes in number peptide detection, x-axis) will have the same color. The following figures expand this overview into a detailed figure for each sample property, those visualization are designed to further dive into each experimental condition and provide respective color legends.

Note that the visualization of sample metadata in this report depends on user-provided input; each column in the metadata input table (besides sample names) that contains more than 1 unique value is automatically used as a factor for color-coding all figures in this section. So the data used for color-coding is also available in the output table 'samples.xlsx'.


detection rates per sample color−coded by sample metadata

color-coding sample metadata, expanded

To further detail each sample property, each row in the above figure is now split into separate plots. Thus, a figure is generated for each experimental condition from the user-provided metadata (column in the samples table, it's name shown in the plot title).

The y-axis shows all unique variables, the x-axis the number of detected peptides and each dot is a sample. The vertical line indicates the median value for each row. Colors are consistent with the above plot.

For example: the first plot shows color-coding by the 'group' property, so each row represents a sample group. If samples in a particular group systematically yield fewer peptides than another group, a clear pattern will be visible.

Note that the *exclude* metadata is a user-provided indication of 'outlier samples' in the dataset that are excluded from downstream statistical analysis.

sample metadata used for color−coding: group
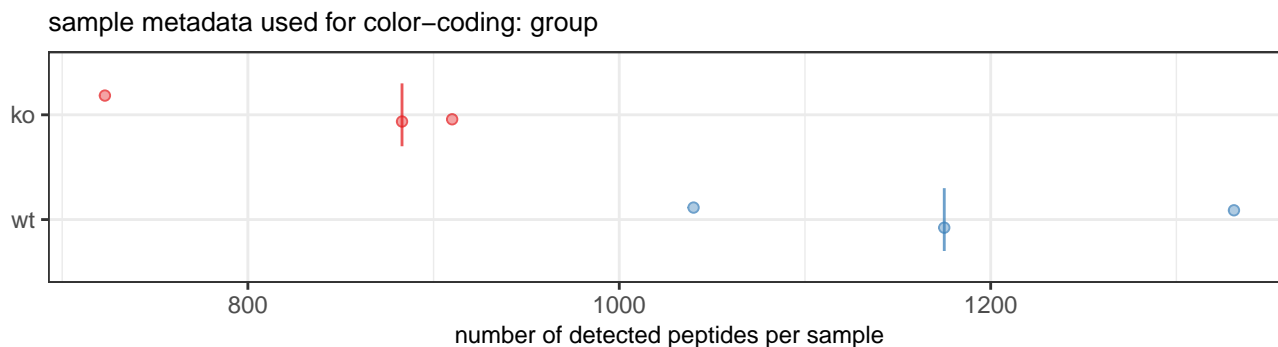
1.2 data completeness

To visualize how many peptides are consistently identified in multiple samples, the first figure summarizes how common missing values are in the entire dataset. Optimally, most peptides are identified in 100% of samples and this curve slowly falls of. The following figure shows for each sample whether its peptides are also present in other samples in the dataset or whether these are unique to a (minor) subset of samples. You can use this mark of experimental consistency to compare datasets generated by similar protocols and mass-spec acquisition.

1.2.1 cumulative distribution
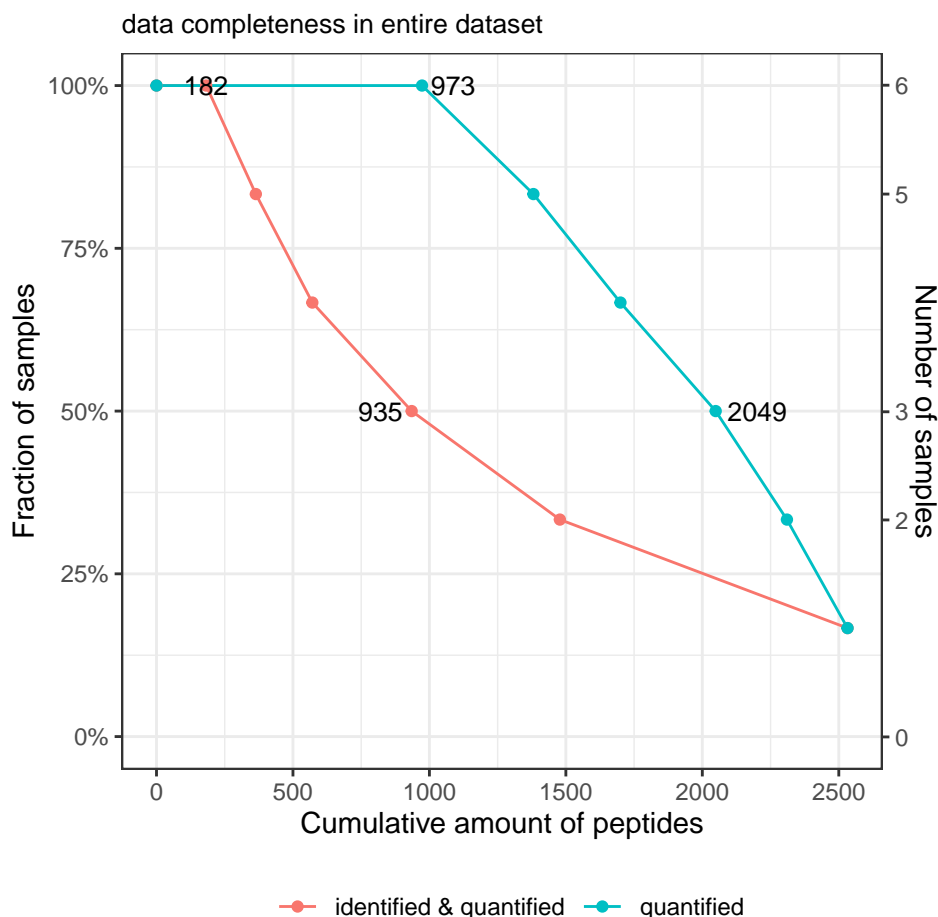
Samples flagged as 'exclude' (by user) are not taken into account in this figure. Exact values are shown for data points matching 90% and 50% of samples to convenience comparison between analyses (e.g. before/after configuring 'exclude' samples, or comparing between experiments of similar protocol).

### 1.2.2 peptide detection frequency

Each identified peptide in a sample is classified and color-coded by the number of other samples where the same peptide is present. Visualization of the amount of peptides that overlap with other samples in the dataset, from peptides identified in most samples (red) to one-hit-wonders (blue), helps identify uncommon samples (more blue/green than other samples).

Optimally, the majority of peptides in each sample are red~orange with relatively few uniquely identified peptides (blue~green). Samples are sorted by the total amount of detected peptides.

Number of samples in which a peptide is identified vs presence in individual sample
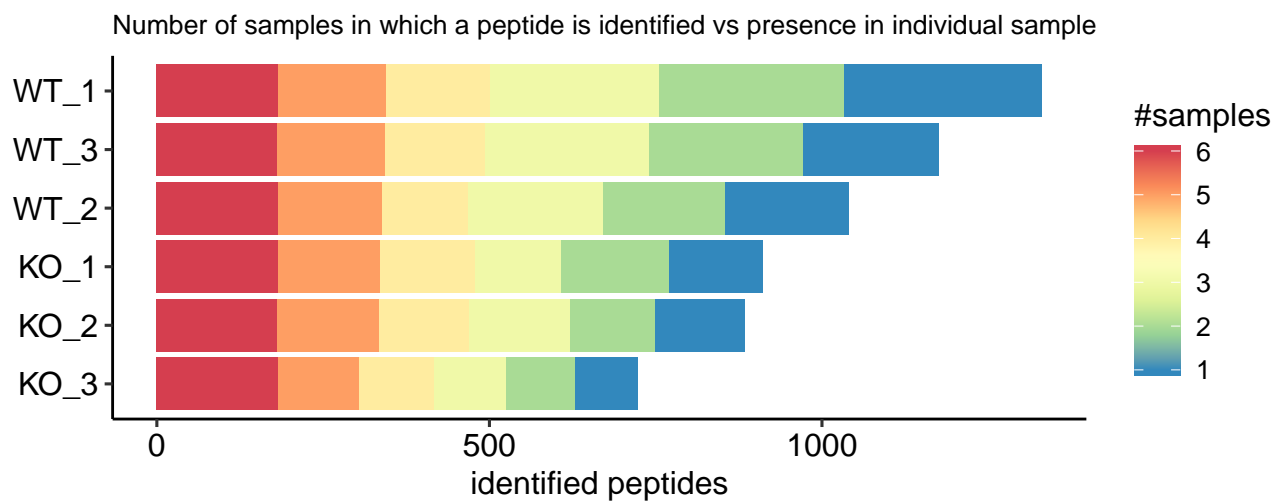
1.3 abundance distributions

The figures in this subsection are used to identify unexpected mass-spec sensitivity or sample loading differences. Peptide data is shown as provided in input files, so peptide filtering nor intensity normalization has been applied yet (for proper QC, make sure the software that generated the input data did not apply normalization prior). If the dataset is DDA, match-between-runs (MBR) peptides are included in these distributions whereas for DIA only 'detected' peptides (based on confidence score threshold) are included.
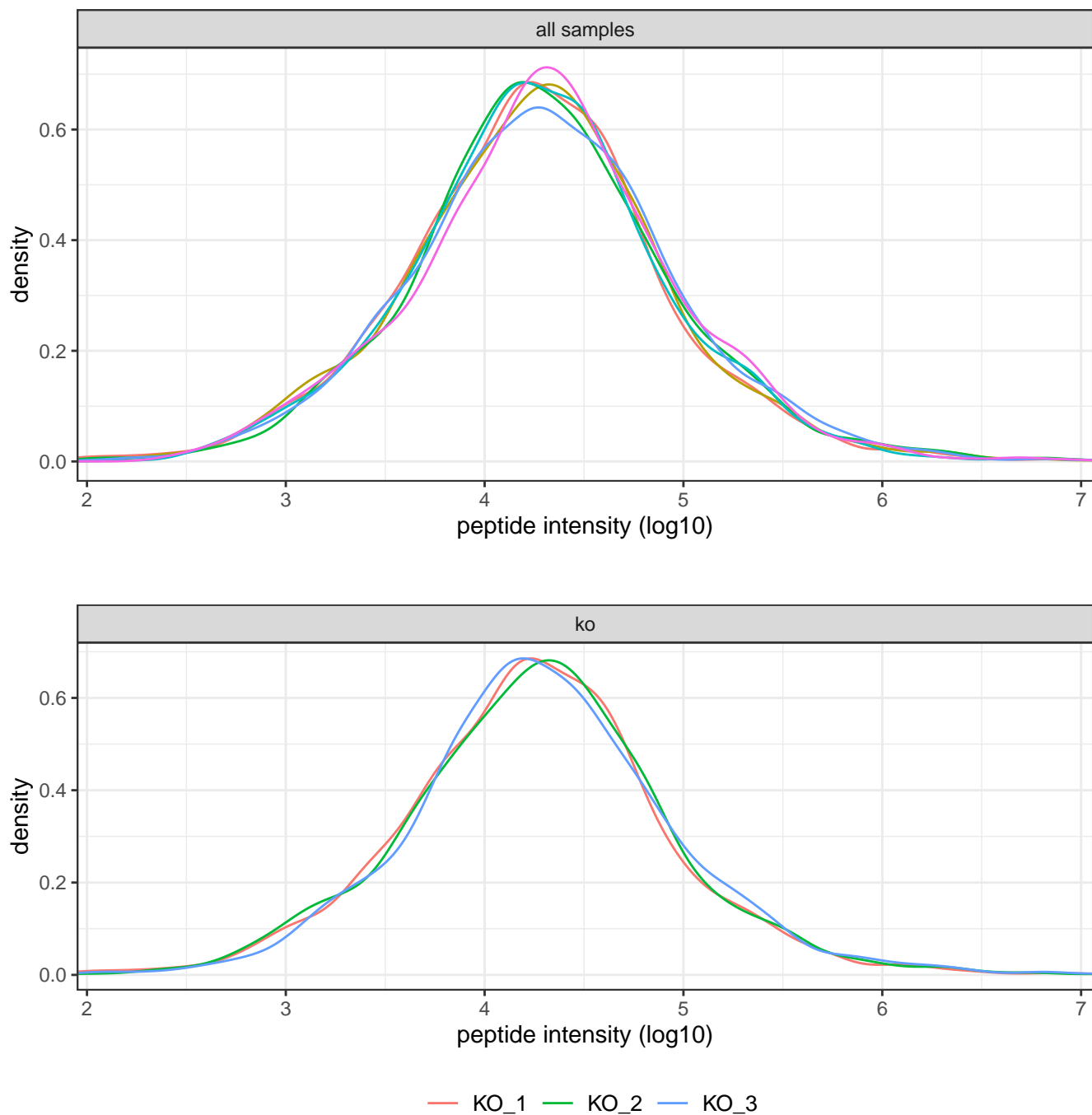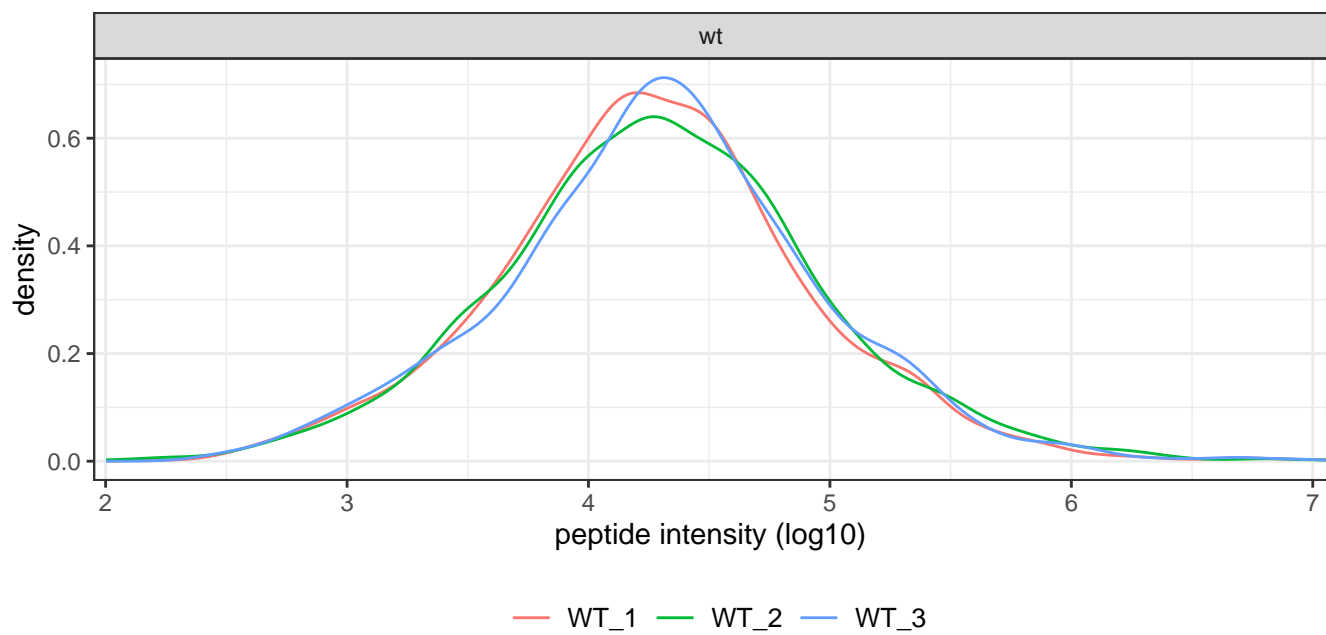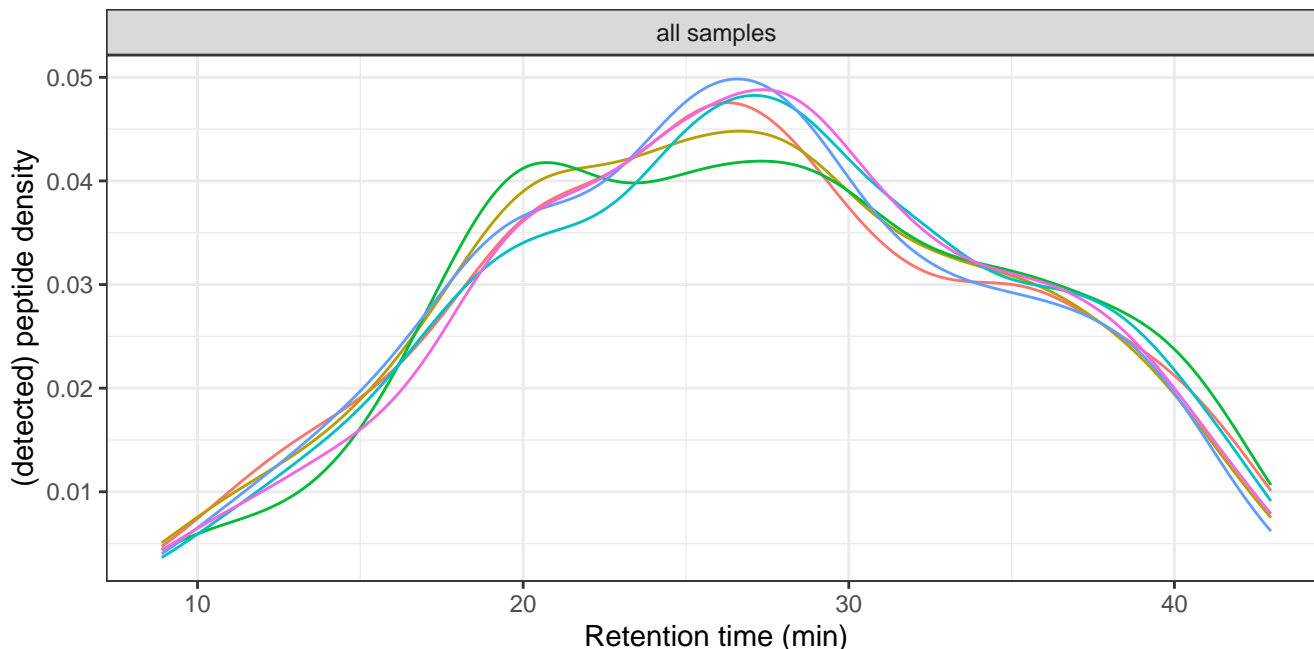
1.4   retention time

The figures in this section allow you to identify potential problems during HPLC elution, such as a temporarily blocking column, failing ionization spray or decreasing sensitivity over time. For each sample, all peptides that are also observed in a replicate (such that there is a point of reference available) are visualized.

1.4.1   retention time distributions

The density of the number of peptides eluting at each point in time. The figure below presents an overview of all samples that allows for the identification of outlier samples that follow distinct elution patterns. The following section shows details for each sample. Samples marked as 'exclude' in the provided sample metadata table are visualized as dashed lines.

progress: RT plots: preparing data took 1 seconds progress: RT plots: creating plots took 1 seconds


1.4.2   retention time local effects

To investigate how each measurement differs from others, we visualize each sample as a 3 panel figure. First, the data is binned across the retention time dimension (x-axis). If a samples was marked as 'exclude' in the provided sample metadata, this is indicated in the plot title.

The top panel shows the number of peptides in the input data, e.g. as recognized by the software that generated input for this pipeline, over time (black line). For reference, the grey line shows the median amount over all samples (note; if this is the exact same in all samples, the grey line may not be visible as it falls behind the black line).

The middle panel indicates whether peptide retention times deviate from their median over all samples (blue line). The grey area depicts the 5% and 95% quantiles, respectively. The line width corresponds to the number of peptides eluting at that time (data from first panel). Analogously, the bottom panel shows the deviation in peptide abundance as compared to the median over all samples (red line).
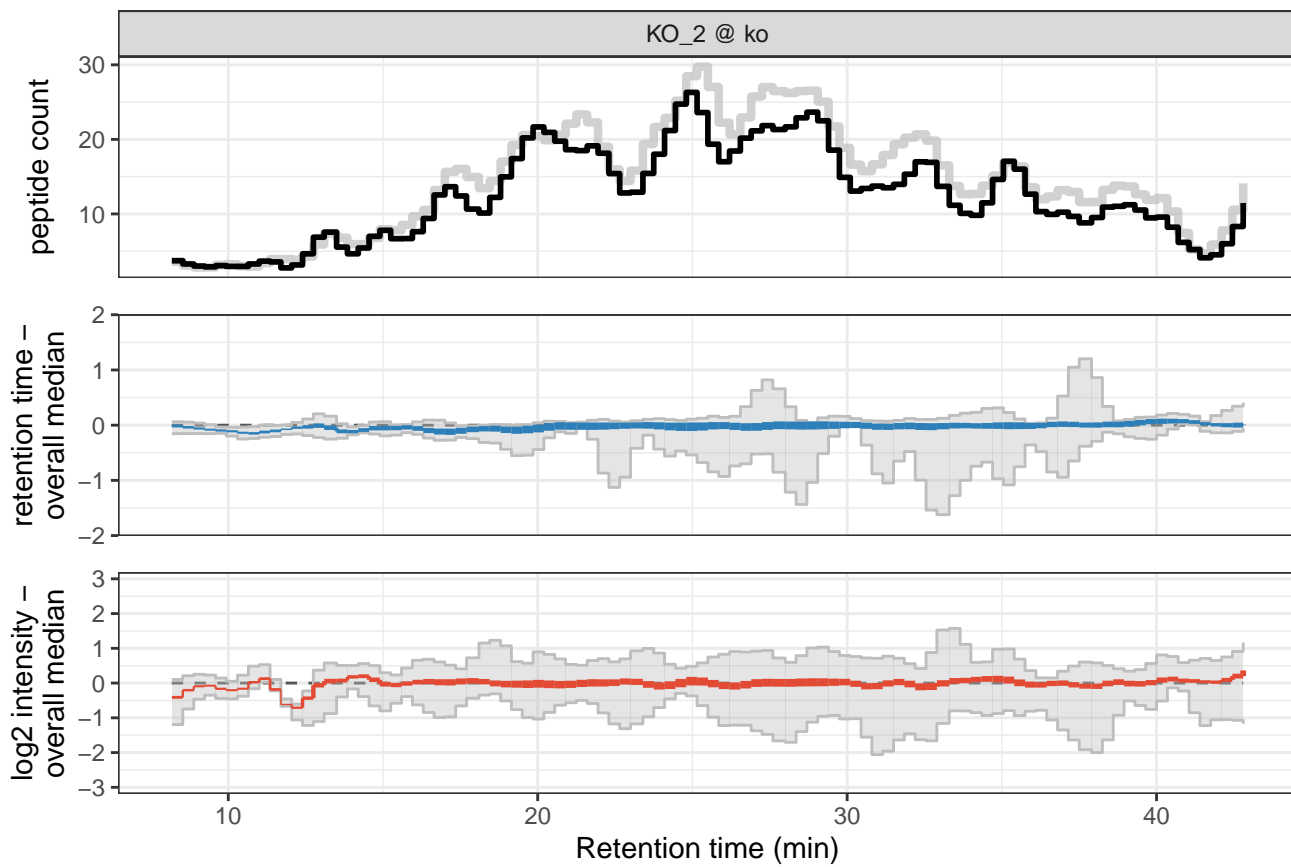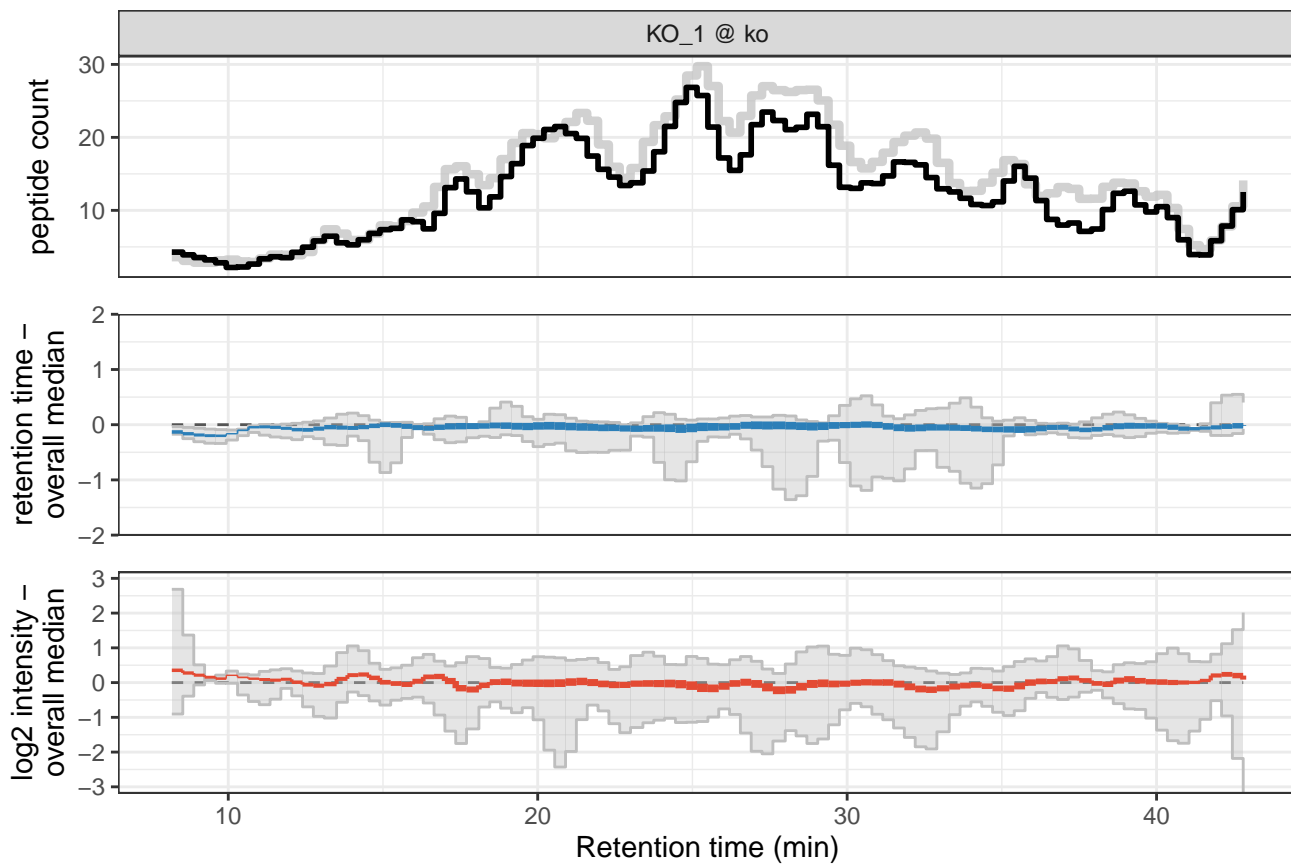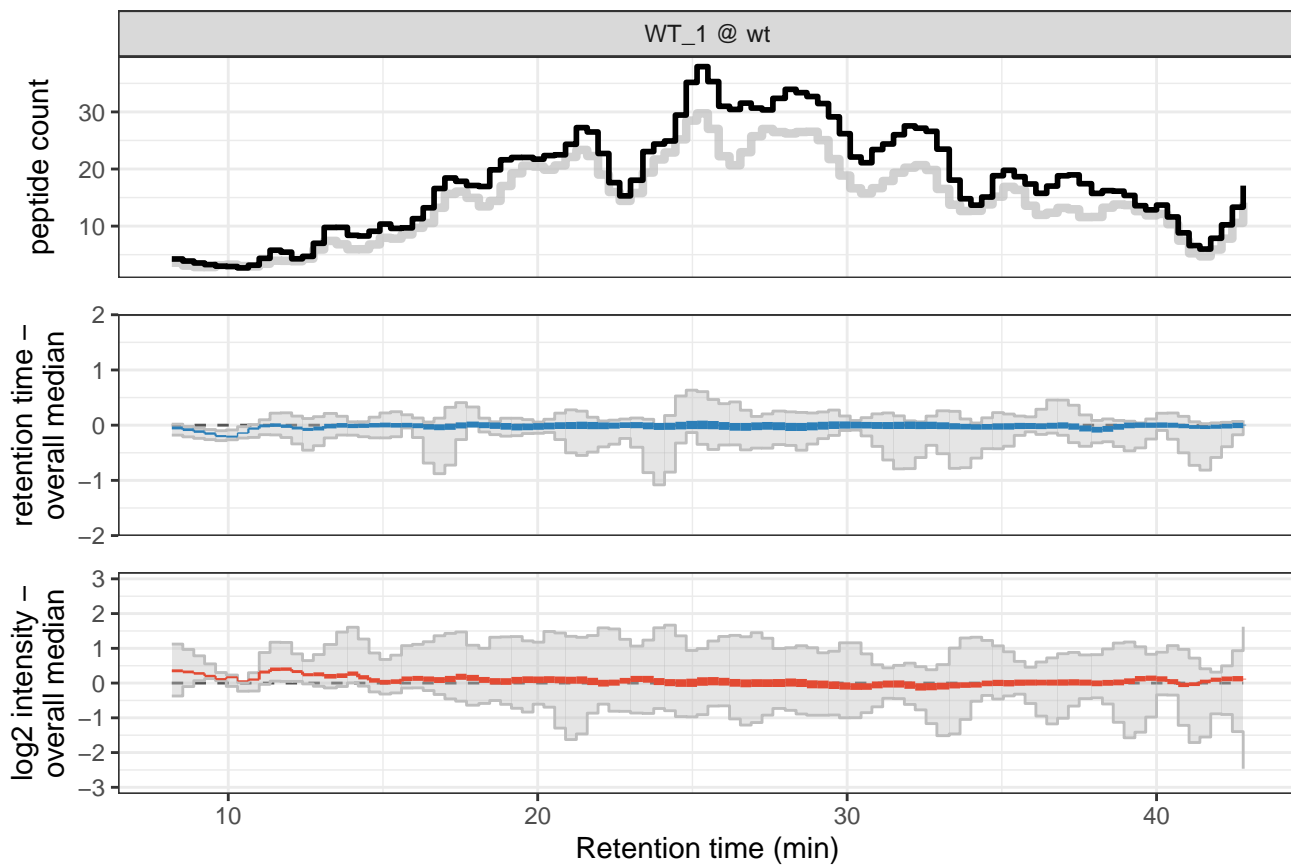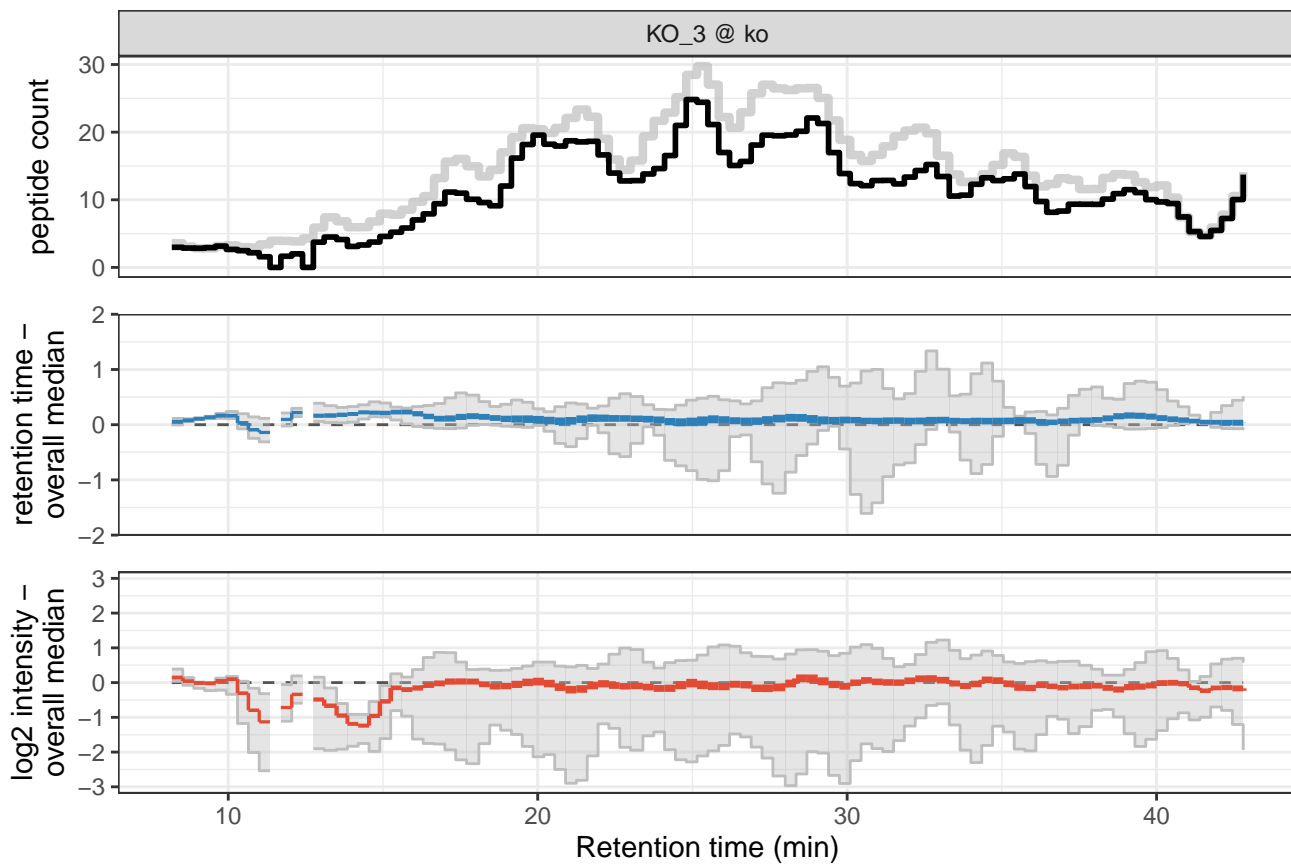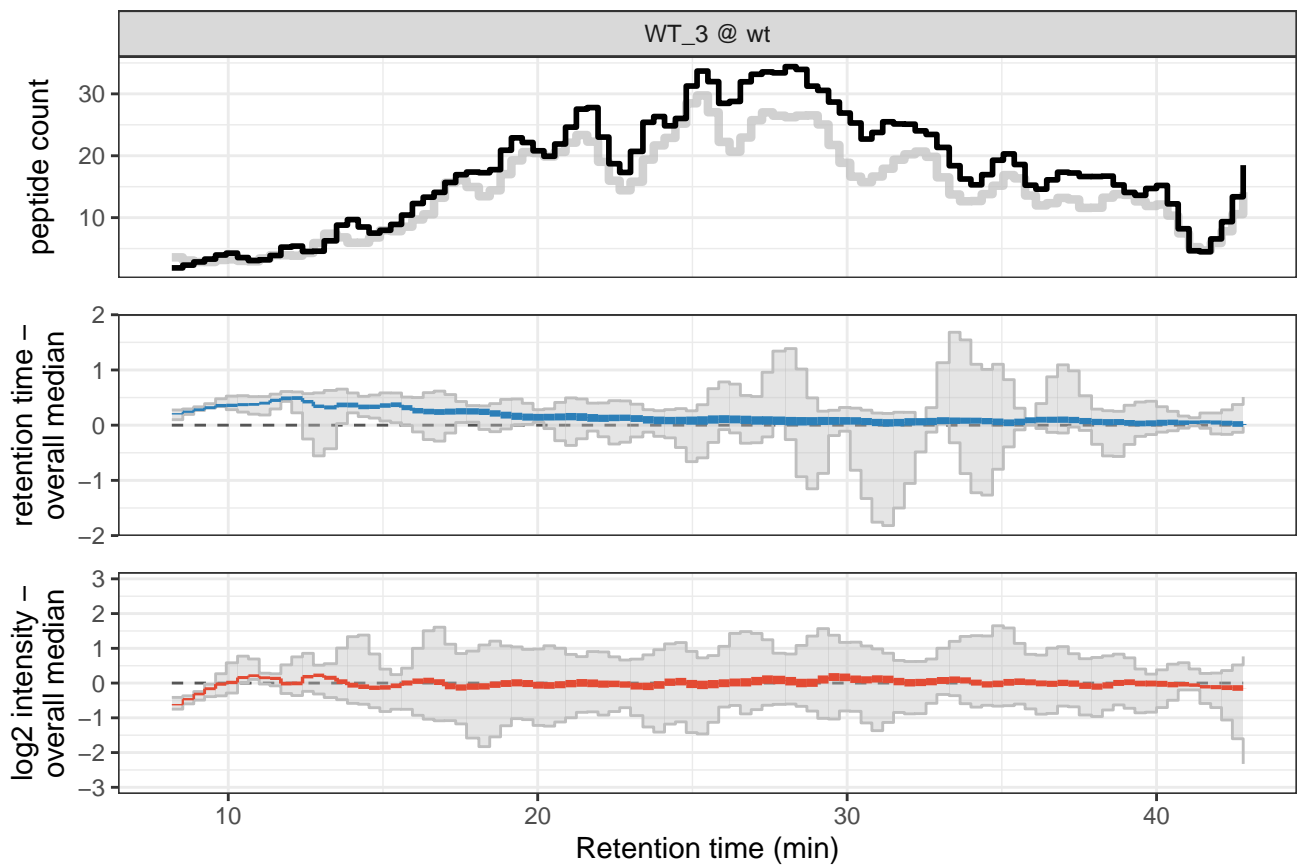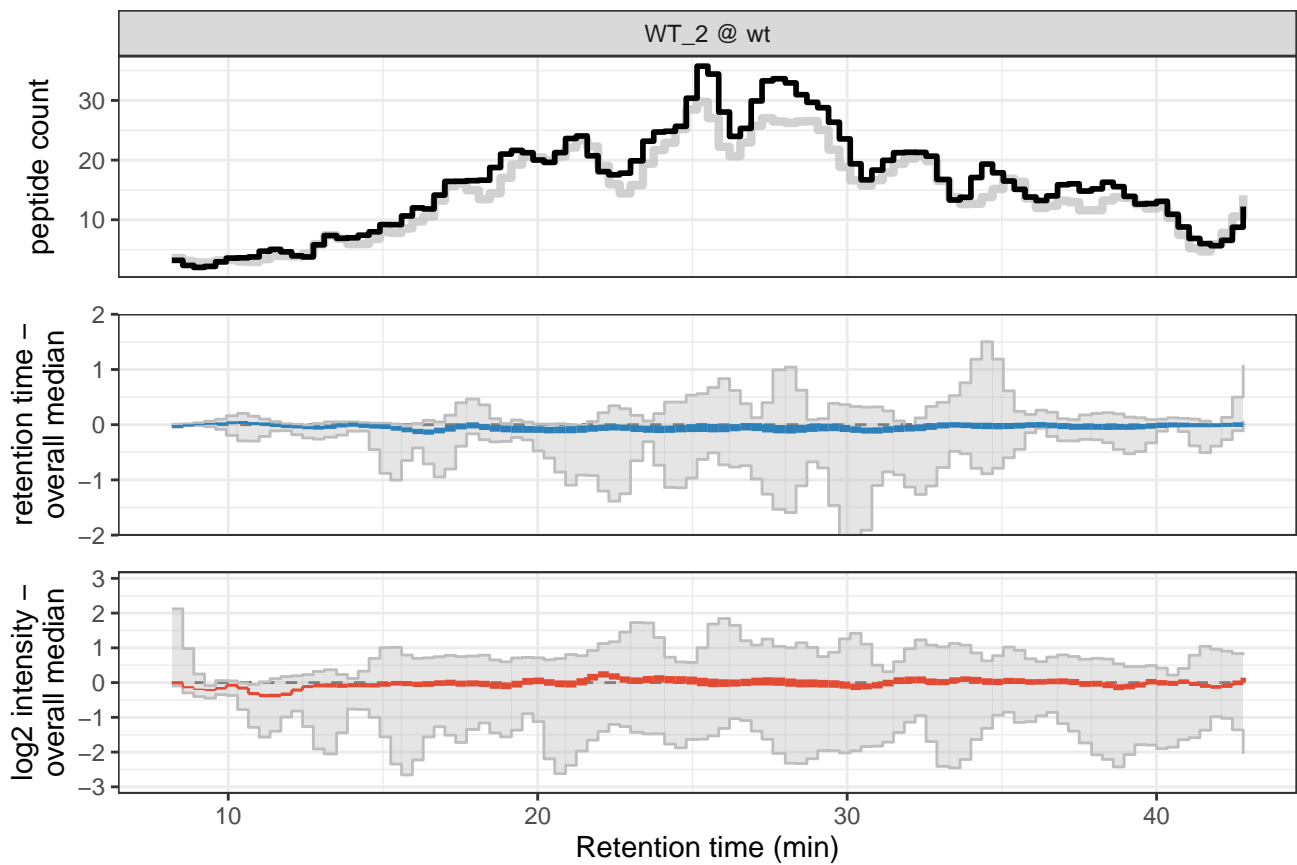
1.5 variation among replicates

The reproducibility of replicate measurements is expressed in three different analyses. First, the difference between peptide intensities in each sample are compared to the mean value among all replicates (foldchange distributions). Next, the Coefficient of Variation (CoV) is used as a metric for reproducibility to explore how much the CoV within a sample group can be improved by removing a single sample (eg; if CoV strongly improved after removing sample s, it could be regarded as an outlier). Finally, the CoV within each sample group is visualized as a boxplot and a violin plot, figures commonly seen in proteomics literature and useful for comparing across experiments (of similar protocol).

1.5.1 within-group foldchange distributions

The foldchange of all peptides in a sample is compared to their respective mean value over all samples in the group. This visualizes how strongly each sample deviates from other samples in the same group which helps identify outlier samples. The same data was used as detailed in the "retention time" section above. Samples marked as 'exclude' in the provided sample metadata table are visualized as dashed lines.
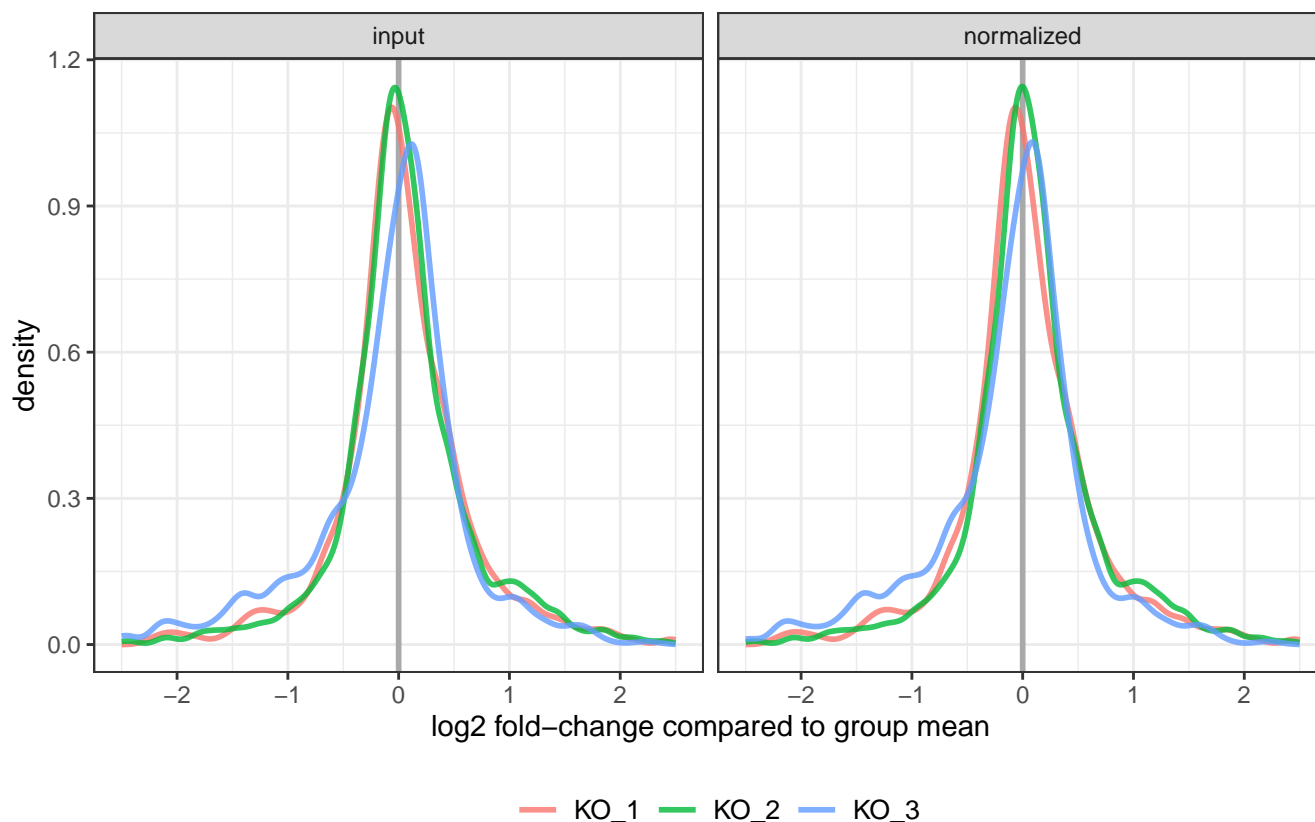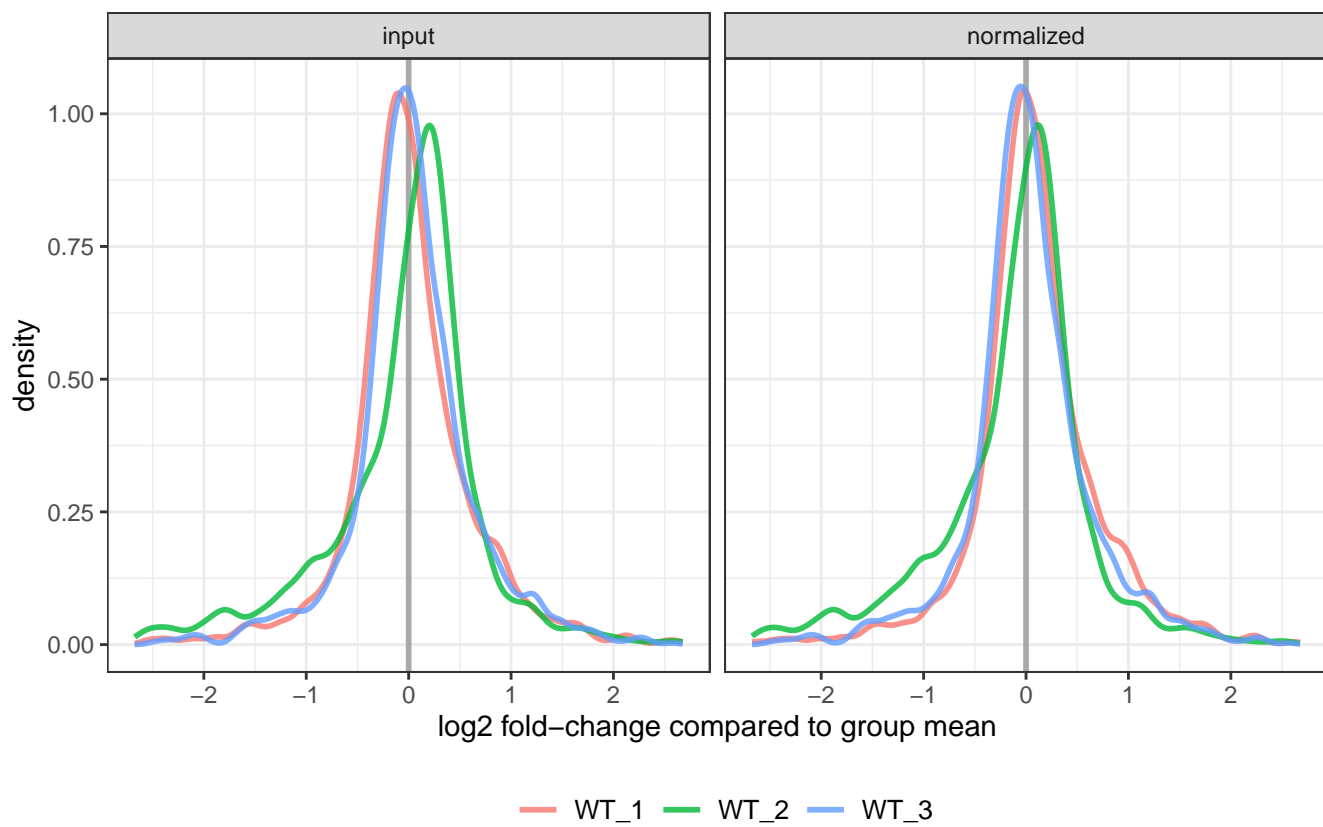
1.5.2   CoV, leave-one-out

No CoV leave-one-out computations could be made, the dataset lacks sample groups with at least 4 replicate samples.

1.5.3 Coefficient of Variation

The Coefficient of Variation (CoV) is a quality metric for the reproducibility of replicate measurements, here visualized using box- and violin-plots.

The same data was used as detailed in the "retention time" section above, with only peptides quantified in at least 3 replicates used for CoV computation in a group. Only samples that are NOT marked 'exclude' in the provided sample metadata and are in a sample group among at least 3 replicates are used for these figures.
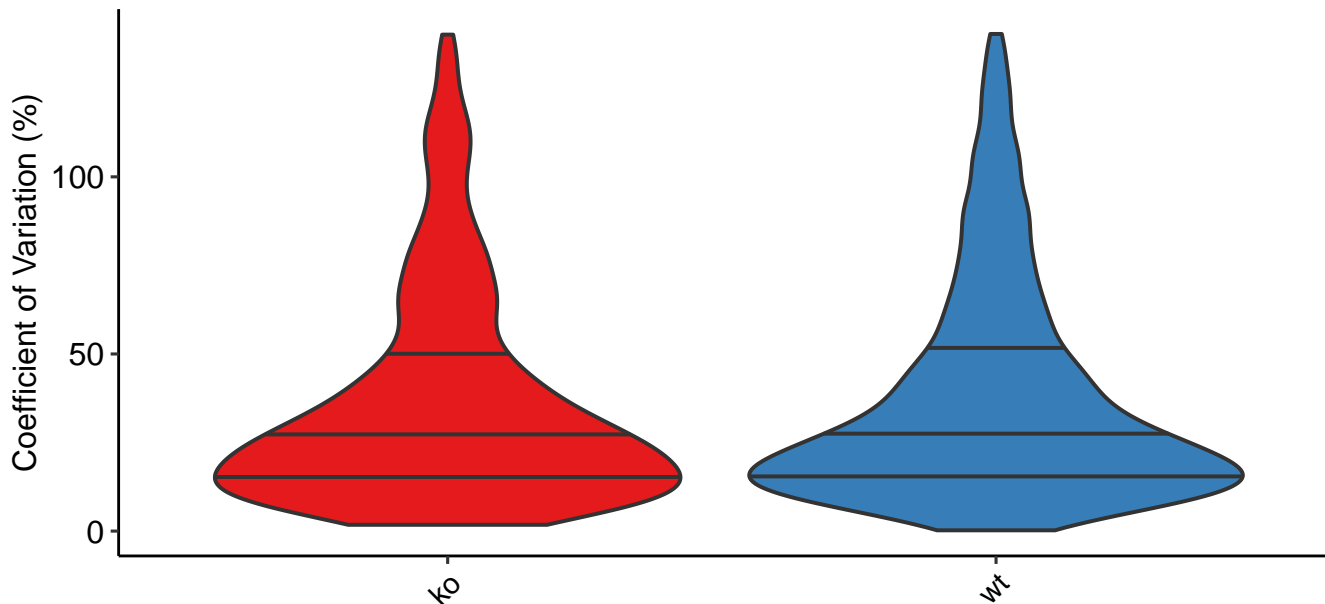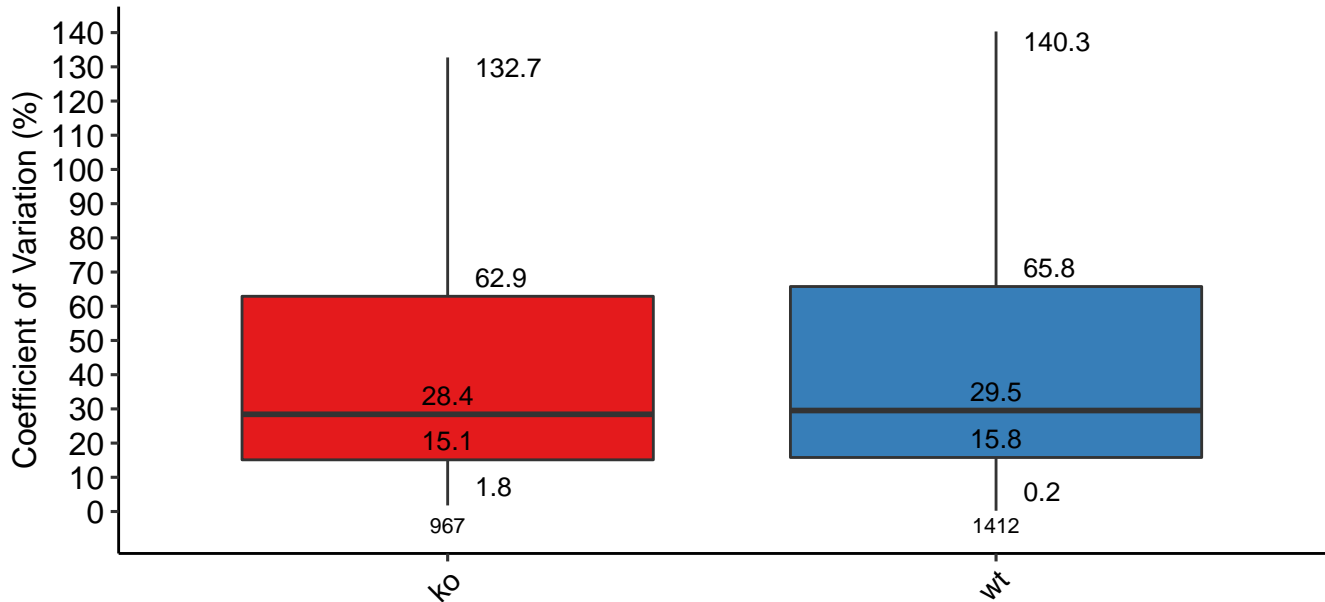
1.6 PCA

A visualization of the first three PCA dimensions illustrates sample clustering. The goal of these figures is to detect global effects from a quality control perspective, such as samples from the same experiment batch clustering together, not to be sensitive to a minor subset of differentially abundant proteins (for which specialized statistical models can be applied downstream).

If additional sample metadata was provided, such as experiment batch, sample-prep dates, gel, etc., multiple PCA figures will be generated with respective color-codings. Users are encouraged to provide relevant experiment information as sample metadata and use these figures to search for unexpected batch effects.

The pcaMethods R package is used here to perform the Probabilistic PCA (PPCA). The set of peptides used for this analysis consists of those peptides that pass your filter criteria in every sample group. If any samples are marked as 'exclude' in the provided sample metadata, an additional PCA plot is generated with these samples included (depicting the 'exclude' samples as square symbols).

Rationale behind data filter
As mentioned above, the aim of the PCA figures is to identify global effects. To achieve this, we compute sample distances on the subset of peptides identified in each group which prevents rarely detected peptides/proteins from having a disproportionate effect on sample clustering. This pertains not only to 'randomly detected contaminant proteins' but also to proteins with abundance levels near the detection limit, which may be detected in only a subset of samples (eg; some measurements will be more successful/sensitive than others).

Figure legends
The first 3 principle components compared visually (1 *vs* 2, 1 *vs* 3, 2 *vs* 3) on the rows. Left- and right-side panels on each row represent the same figure without and with sample labels. The principle components are shown on the axis labels together with their respective percentage of variance explained. Samples marked as 'exclude' in the provided sample metadata, if any, are visualized as square shapes.

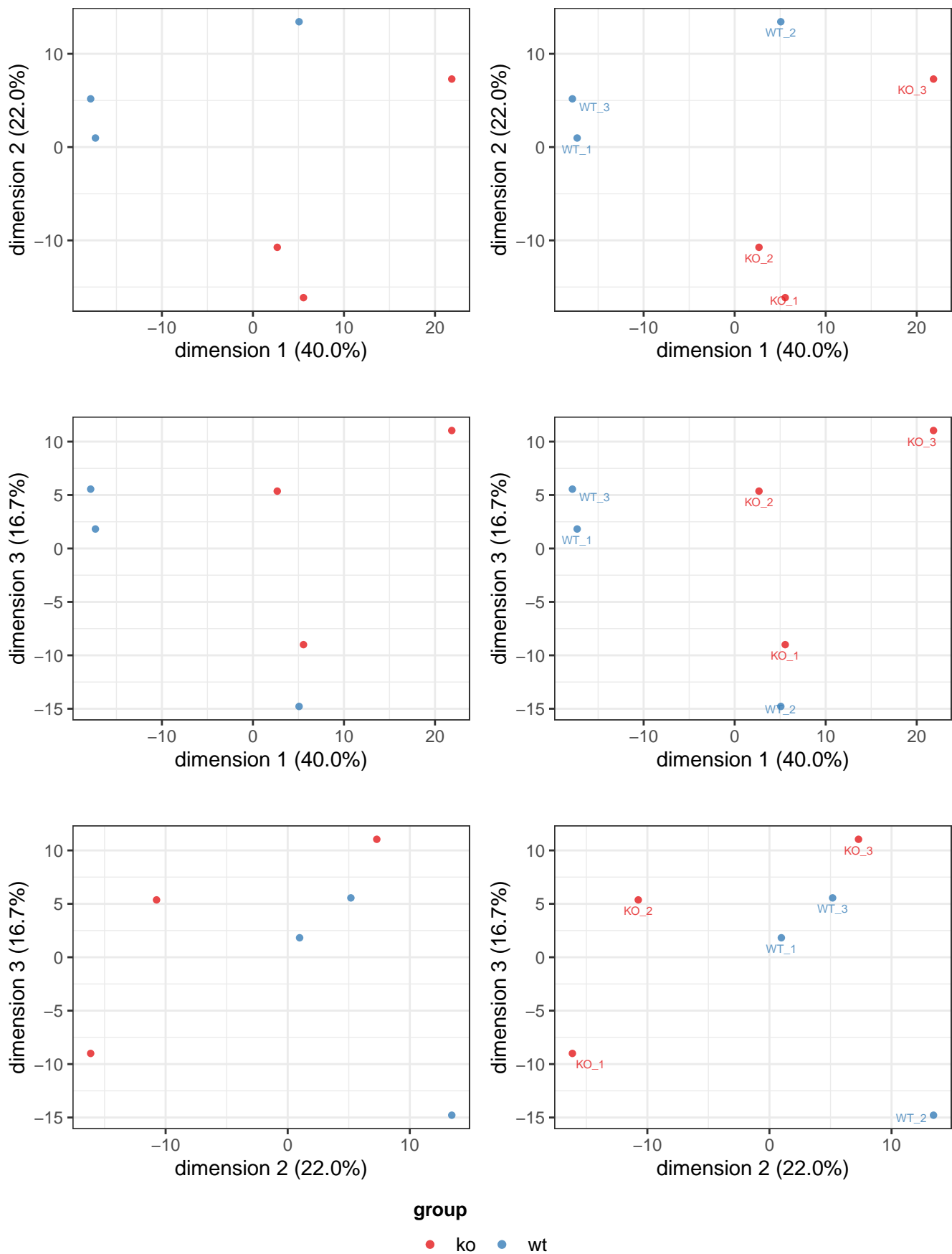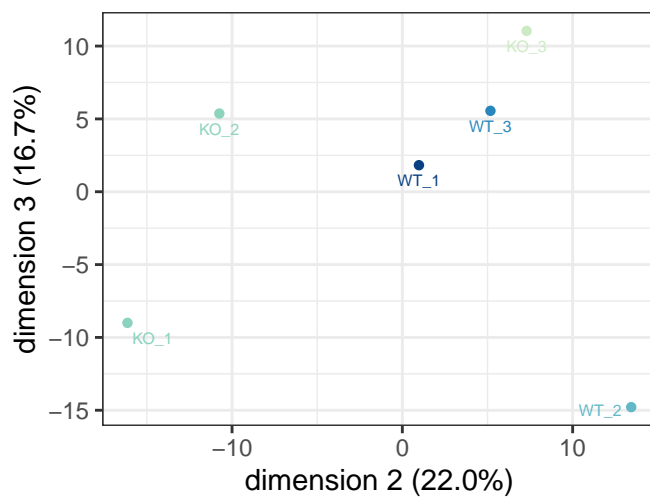**PCA only on samples not flagged as 'exclude', using 716 peptides**
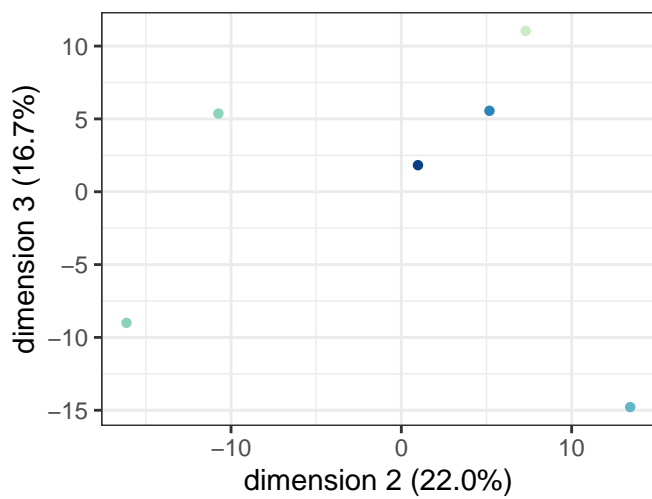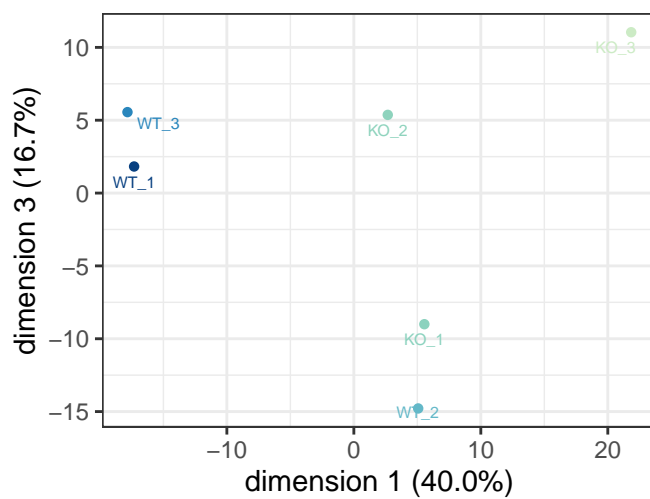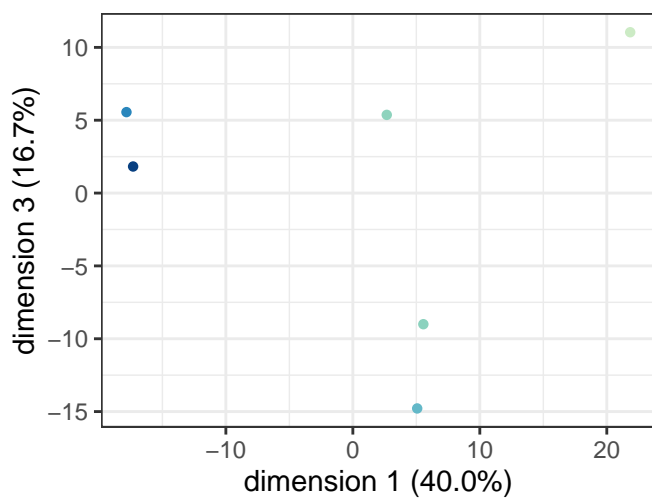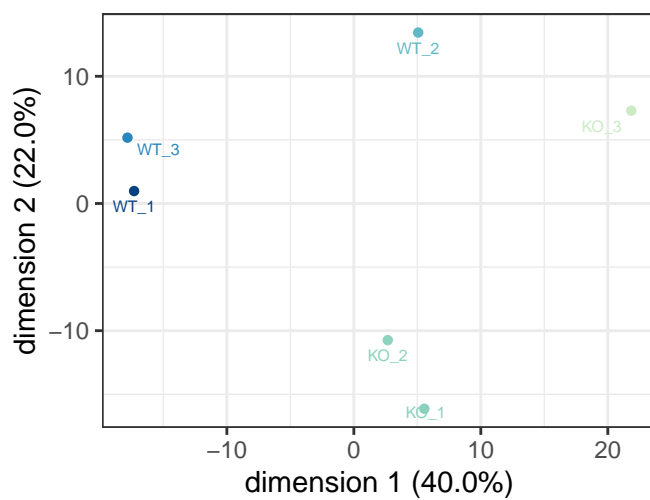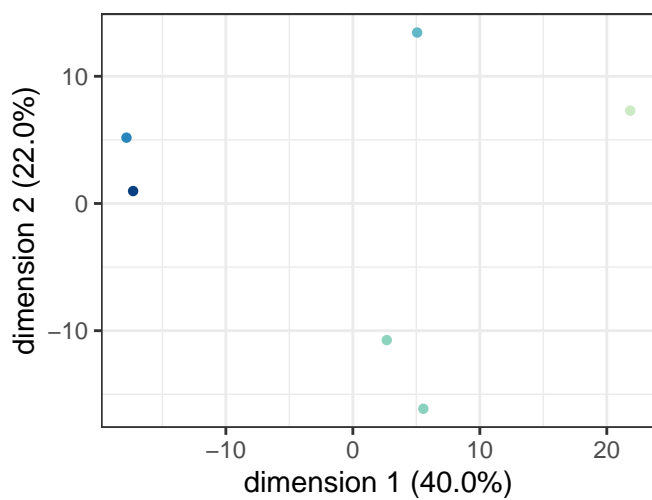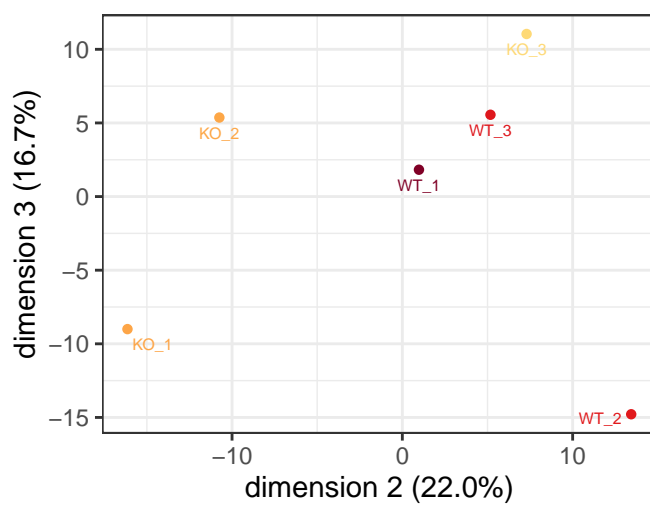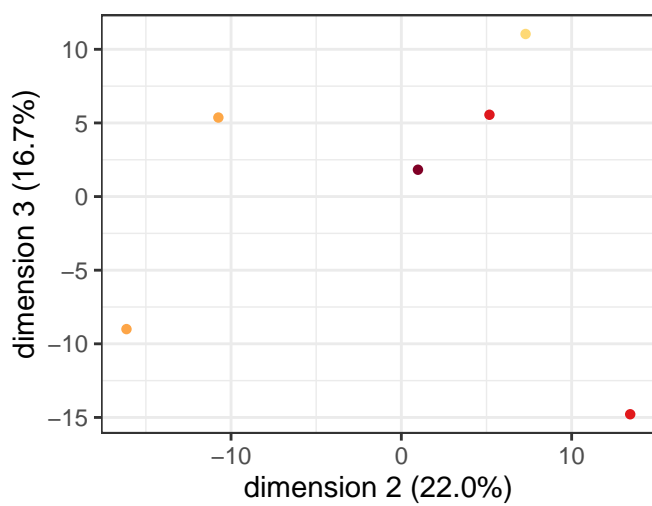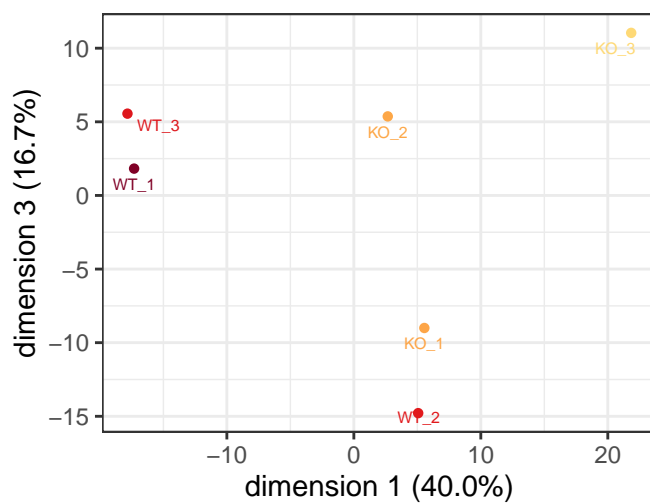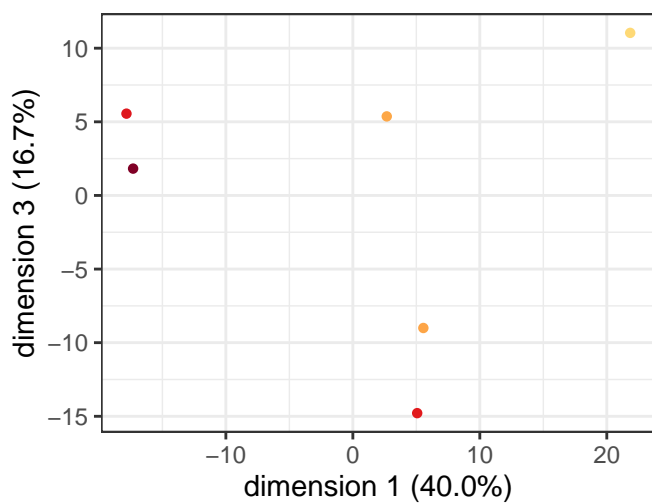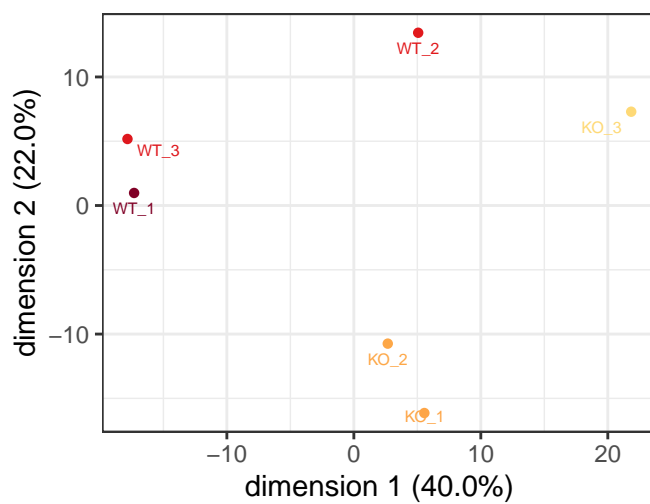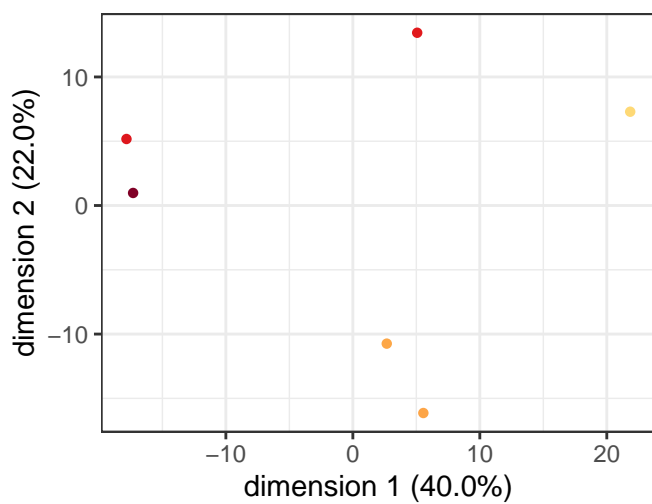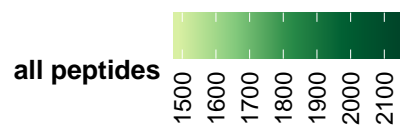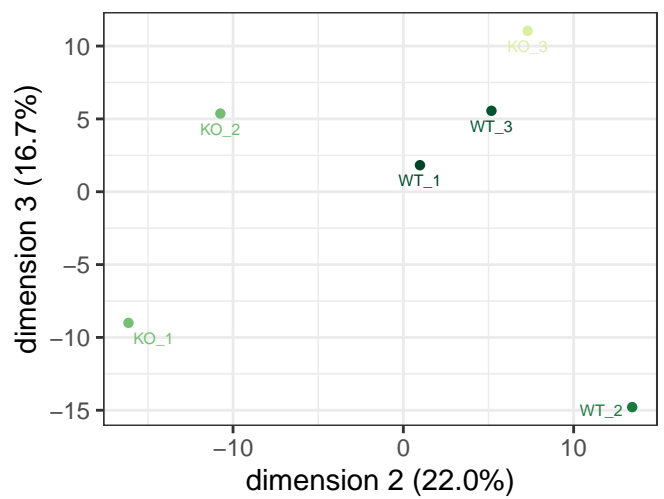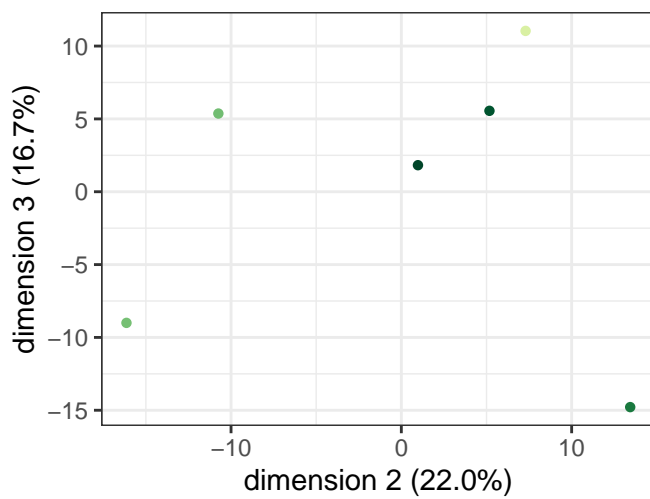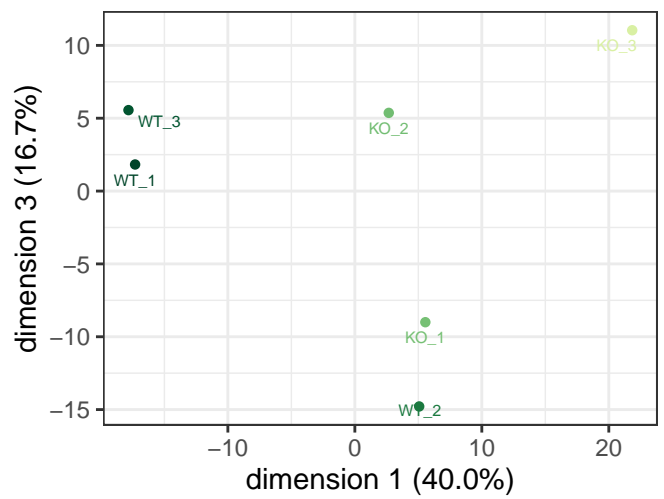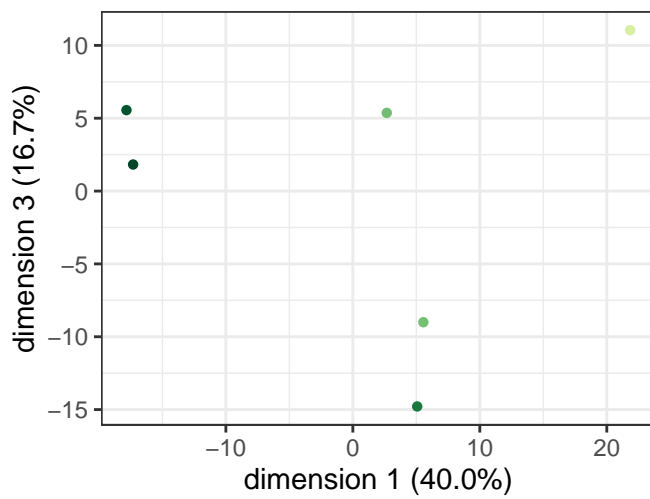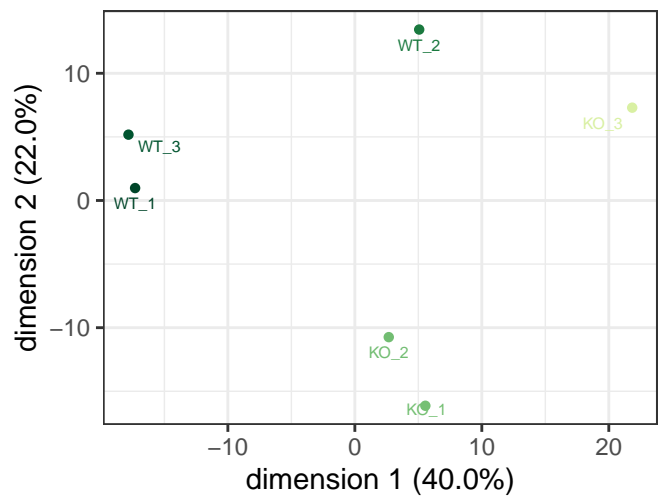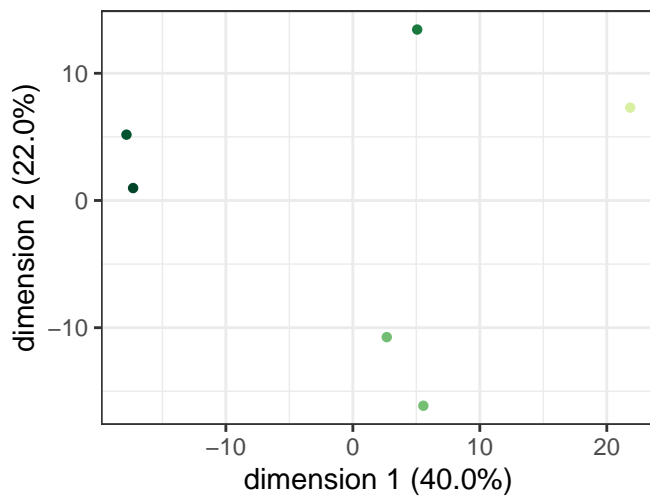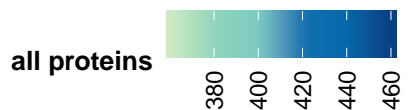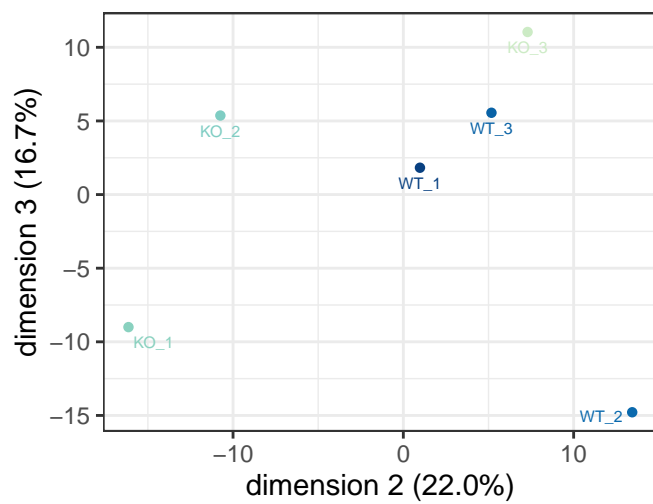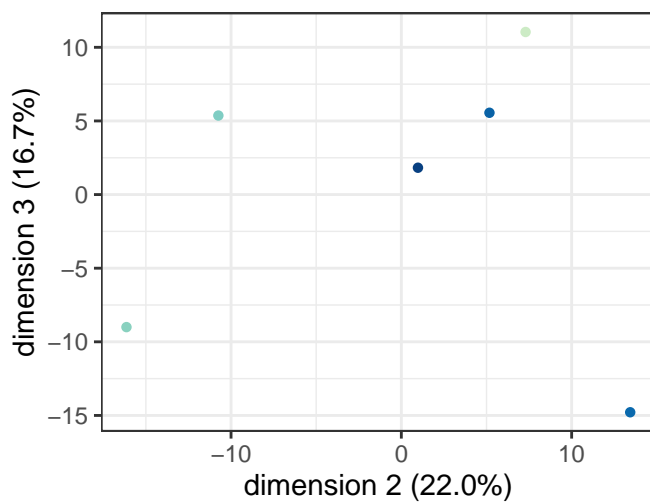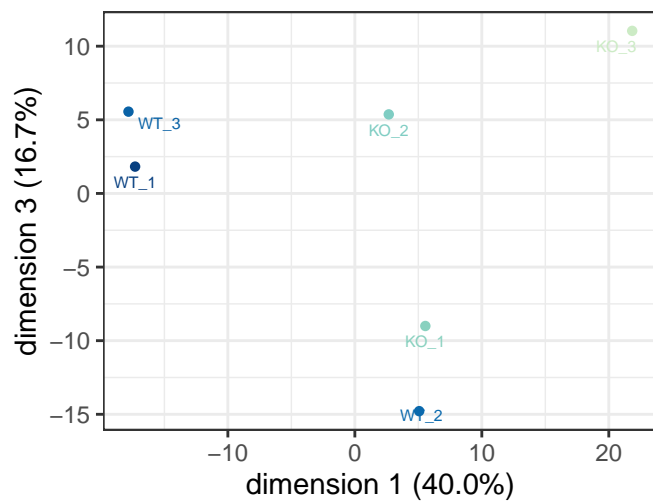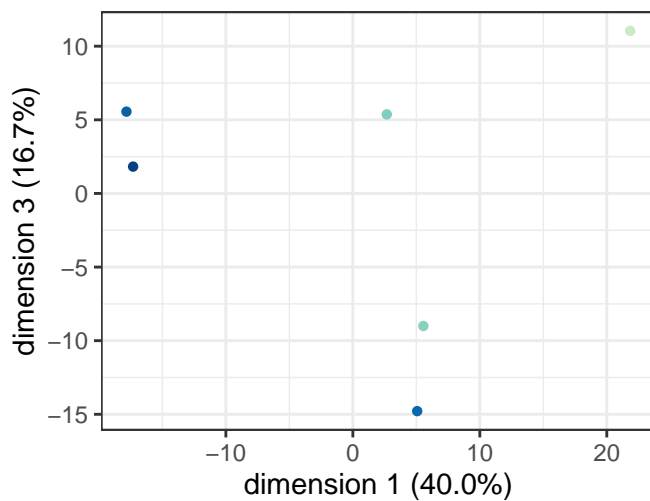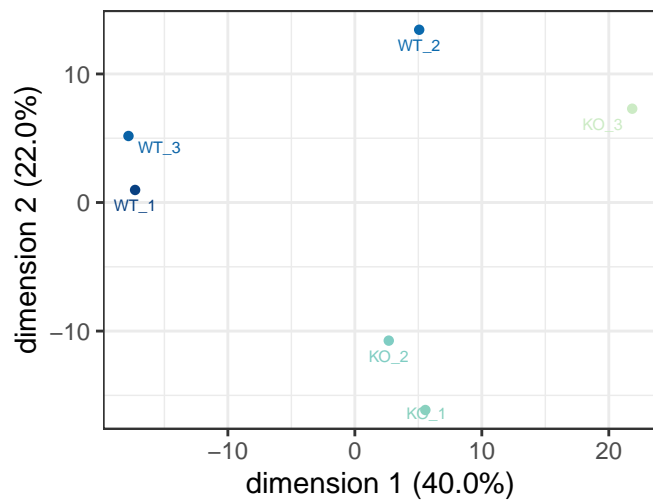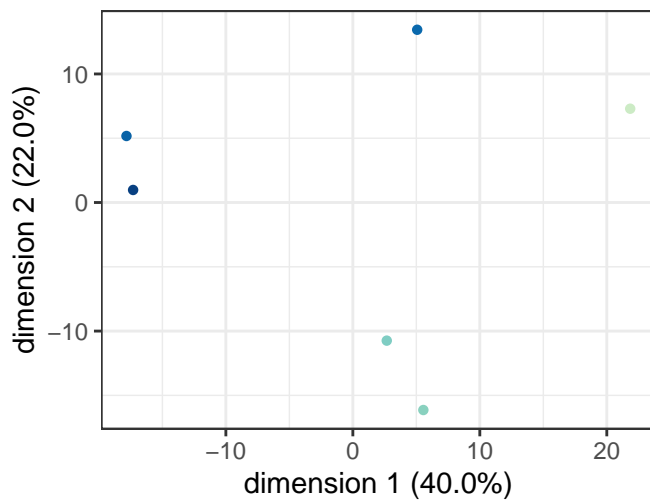
2 Differential abundance analysis

goal: maximize reliable features for quantification

In a pairwise analysis of two groups of samples, only peptides with N data-points in both groups are used for quantitative analysis (where N = defined by user settings). For example; if peptide p is consistently quantified in sample groups A and B but not in C/D/E, it can be used when comparing group A *versus* group B but should not be used in any other group comparisons. This approach is particularly suited to maximize the number of peptides used for statistical analysis in experimental designs with many sample groups.

A common alternative strategy is a global filtering approach where peptides are selected based on their properties in the overall dataset (eg; present in x% of samples or x% of replicates in all groups) and subsequentially the resulting data matrix is used for all downstream statistical analyses. In the example above where peptide p is present in a subset of sample groups, p would either be left out (not present in majority of samples in entire dataset) or erronously used when applying t-statistics to groups B and C (since p is not present in group C, it may differentially detected but there are no features available for quantitative analysis)

2.1 wt vs ko

- **user setting:** using 'global data filter' peptide filtering approach

- 2532 peptides in 541 proteins remain in the current contrast after peptide filters and are used for the statistical analysis in this section

- qvalue threshold: 0.05

- log2 foldchange threshold: 0.9646236

2.1.1 volcano

The plot title shows the statistical model and contrast (sample groups in the comparison). Left- and right-side figure panels on each row represent the same figure without and with labels for the 25 proteins with lowest p-value.

Bottom figure panels have limited x- and y-axis. For datasets with a small number of strong outliers in p-value or fold-change, which may have a profound effect on the plot scales, this allows inspection of the remainder of the volcano plot without disproportionate influence by 'extreme' values.
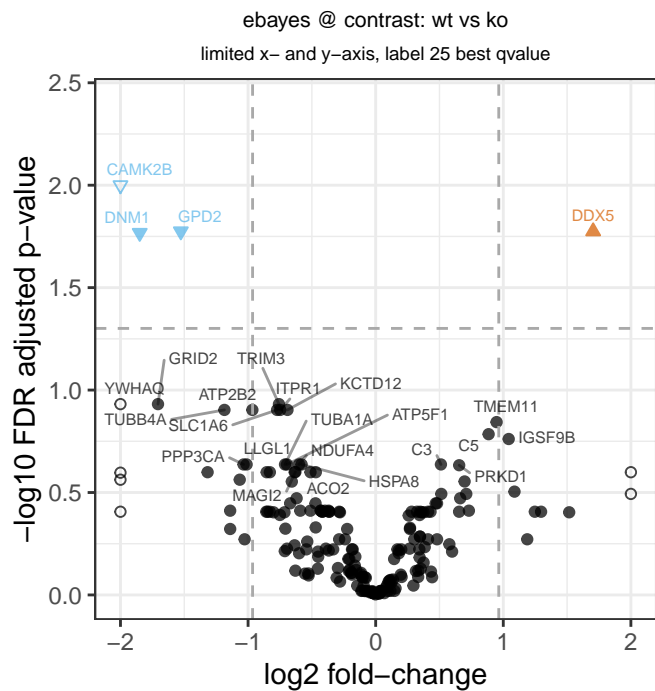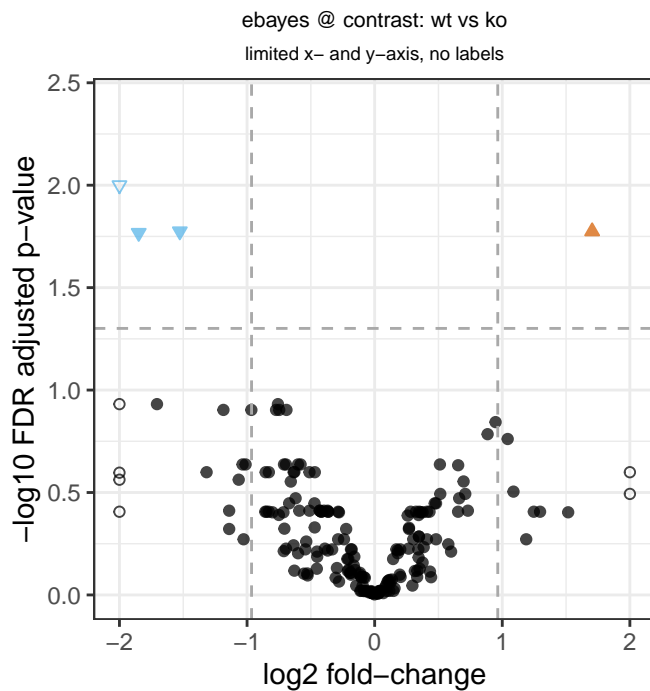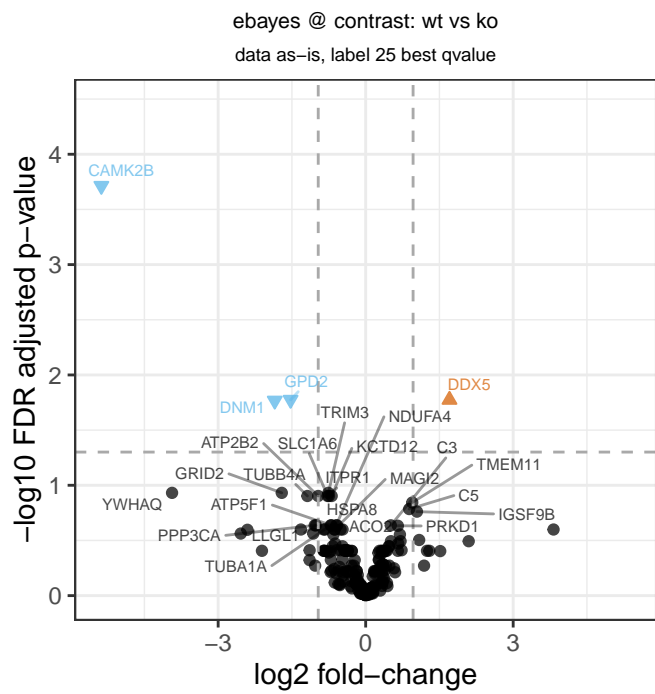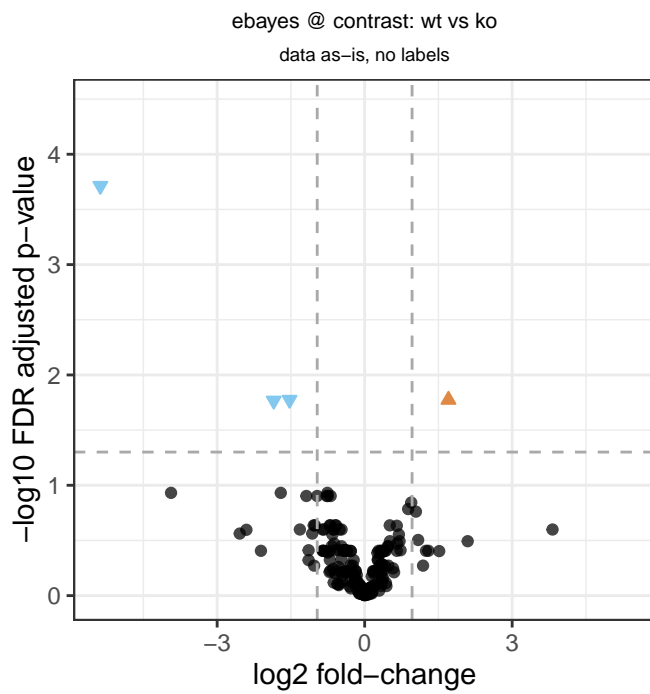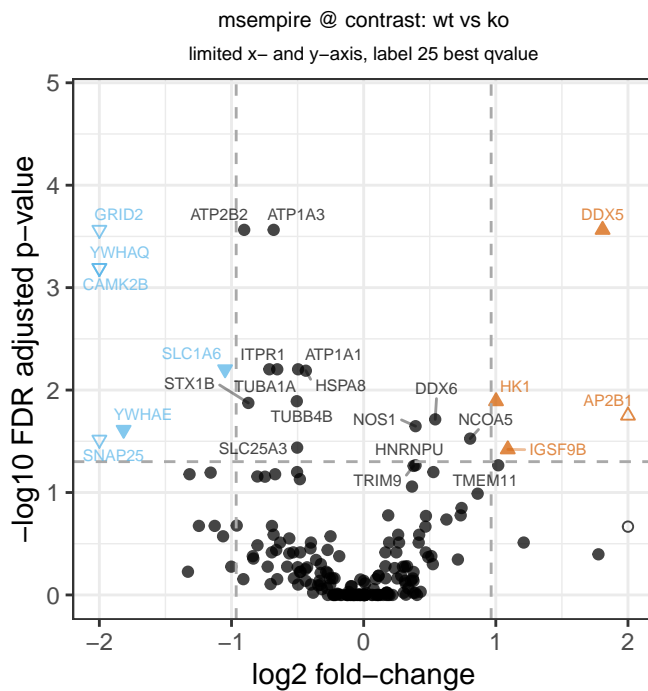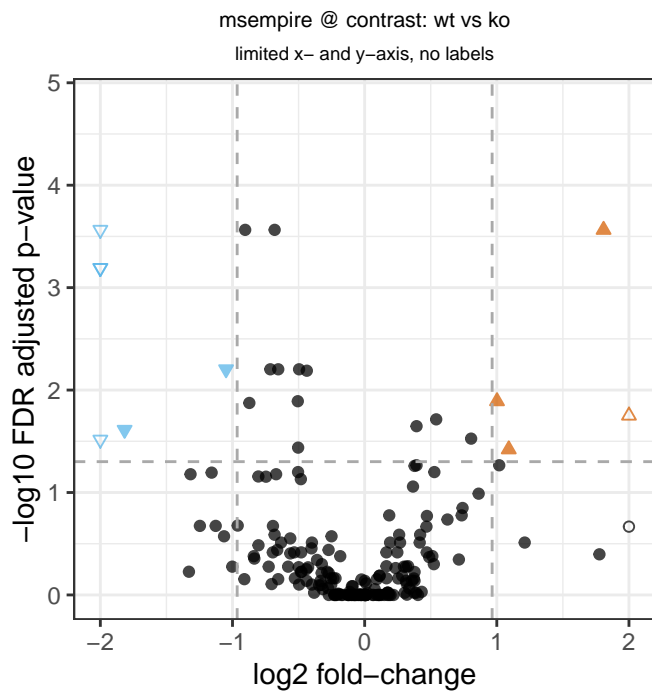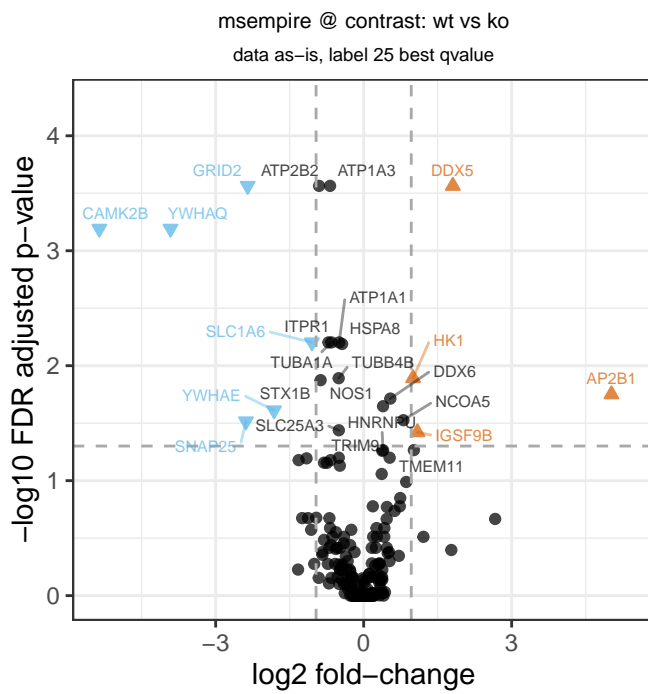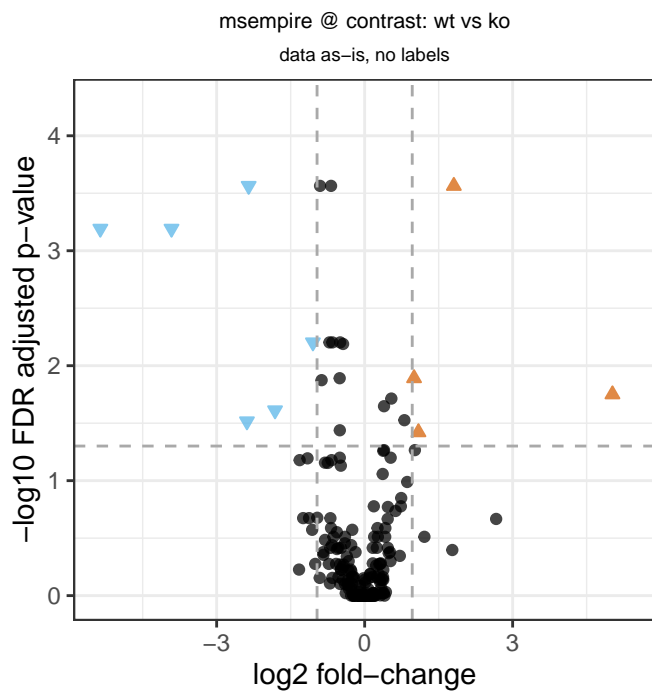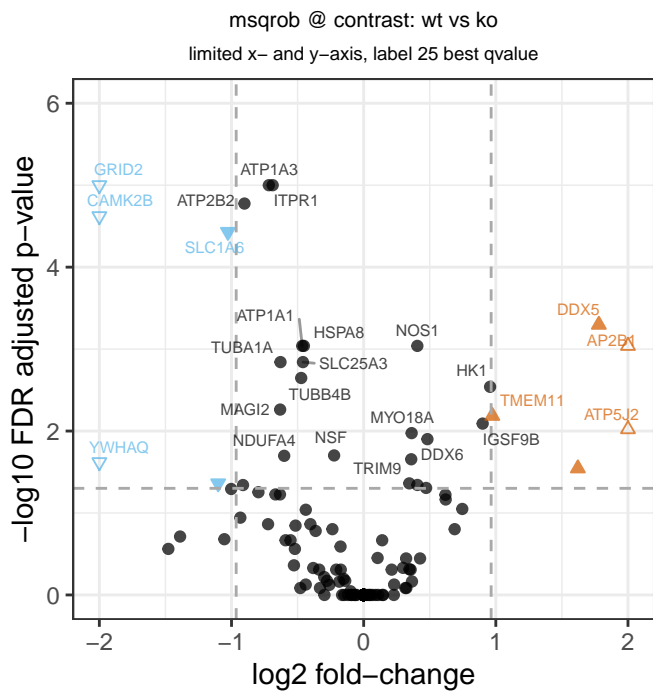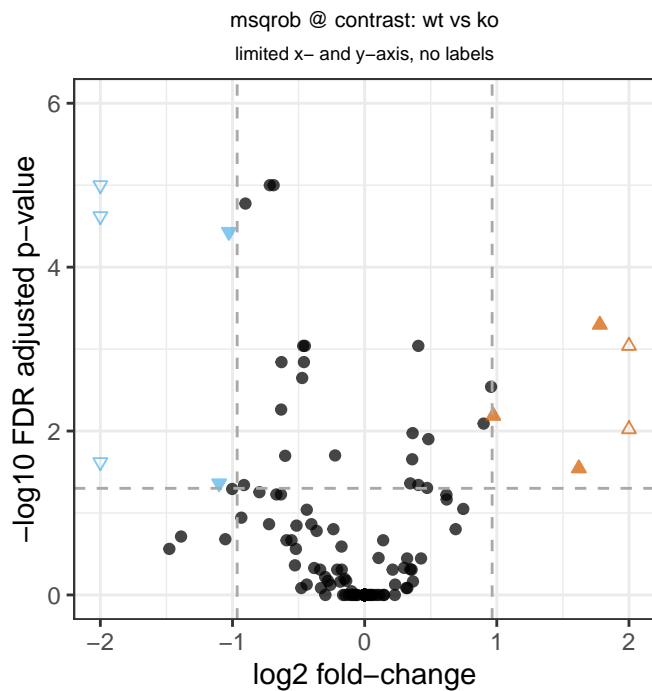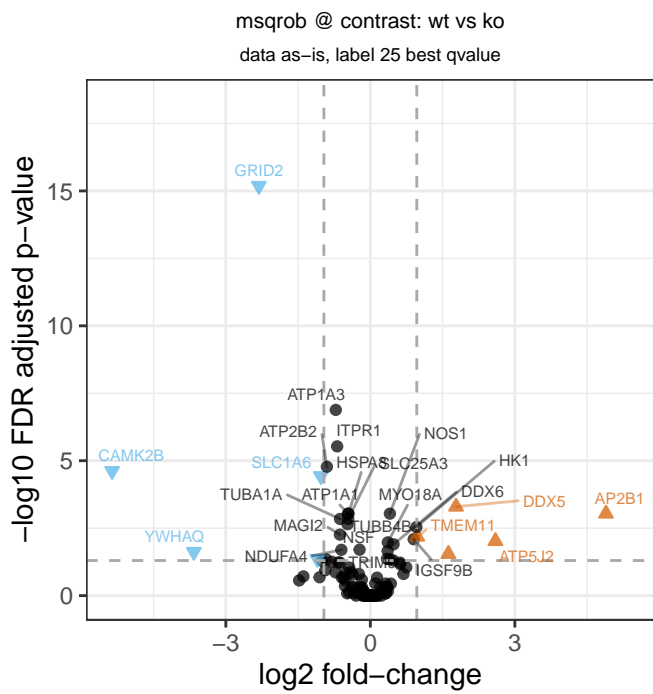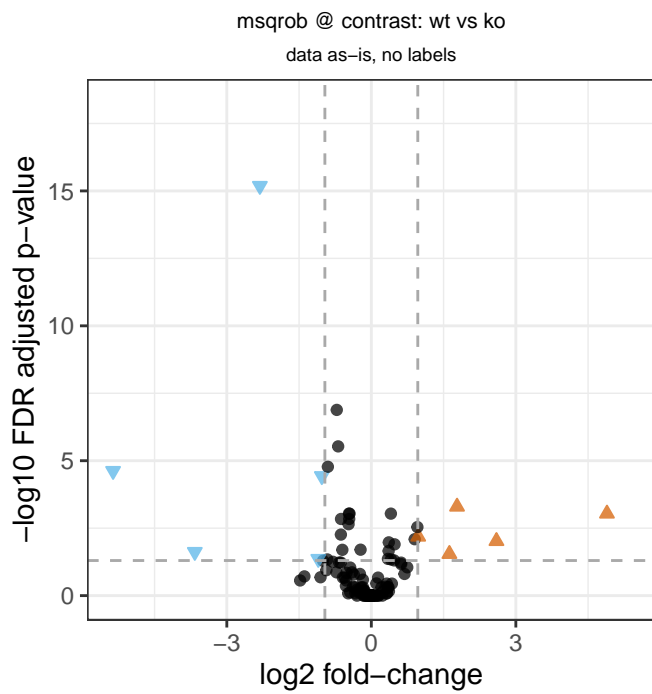
2.1.2 foldchange distribution

Distributions of estimated foldchanges produced by the statistical models. If the mode is far from 0, consider alternative normalization strategies. Do note the scale on the x-axis, for some experiments the foldchanges are very low which in turn may exaggerate this figure.

note; the MSqRob model tends to assign zero (log)foldchange for proteins with minor difference between conditions where the model is very sure the null hypothesis cannot be rejected (shrinkage by the ridge regression model). As a result, many foldchanges will be zero and the density plot for MSqRob may look like a spike instead of the expected Gaussian shape observed in other models

contrast: wt vs ko
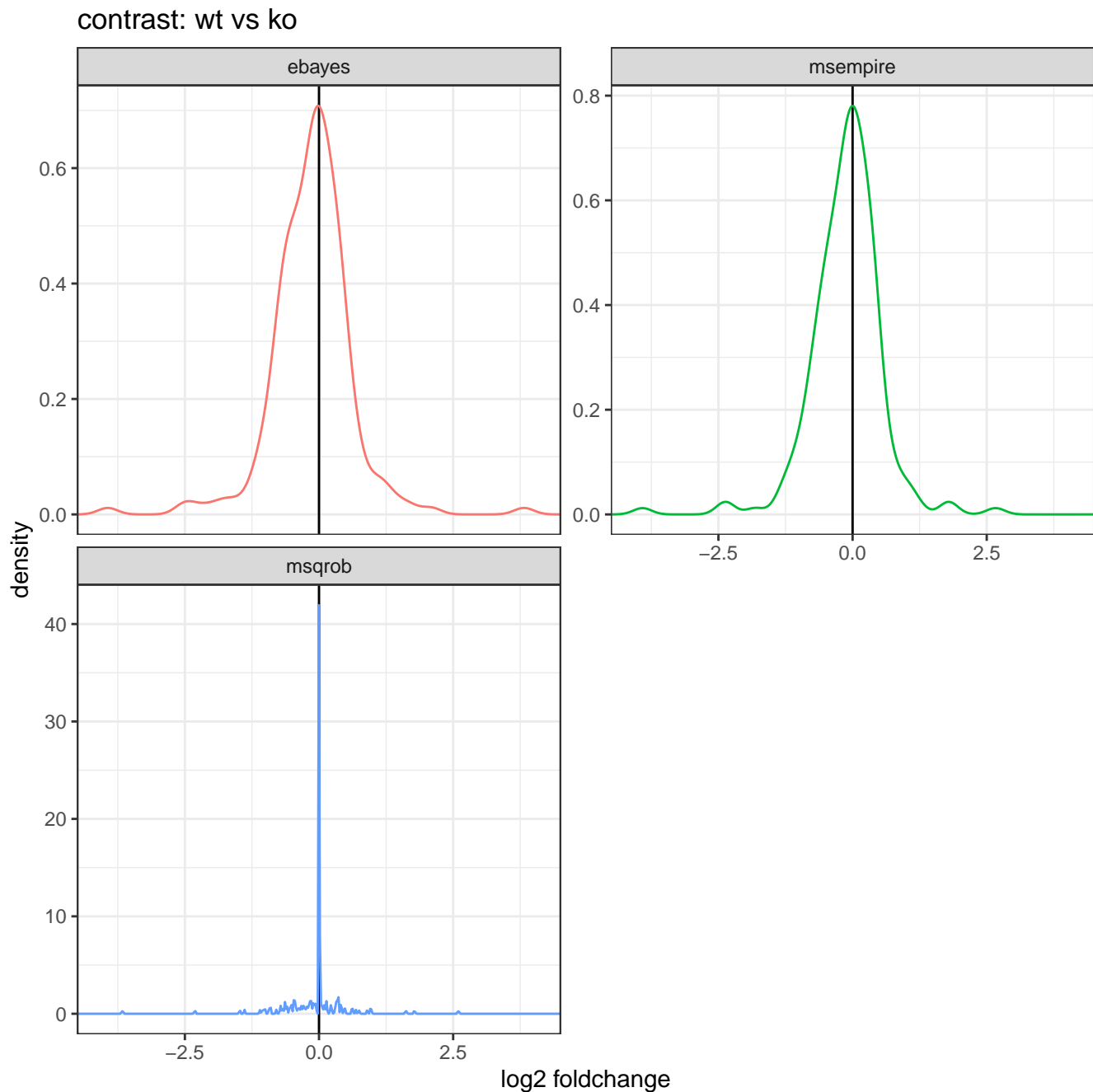
2.1.3 p-value distribution

Histogram of p-values computed by differential expression analysis algorithms, as-is, for quality-control inspection. The horizontal line indicates the expected counts assuming a uniform distribution (total number of p-values divided by number of histogram bins)

See further: https://www.ncbi.nlm.nih.gov/pmc/articles/PMC6164648/

See further: http://varianceexplained.org/statistics/interpreting-pvalue-histogram/

note; the MSqRob and MS-EmpiRe models often yield p-value distributions that show a large peak at p-value 1, these are typically proteins with estimated log foldchanges at/near zero where these models are very sure the null hypothesis cannot be rejected

contrast: wt vs ko
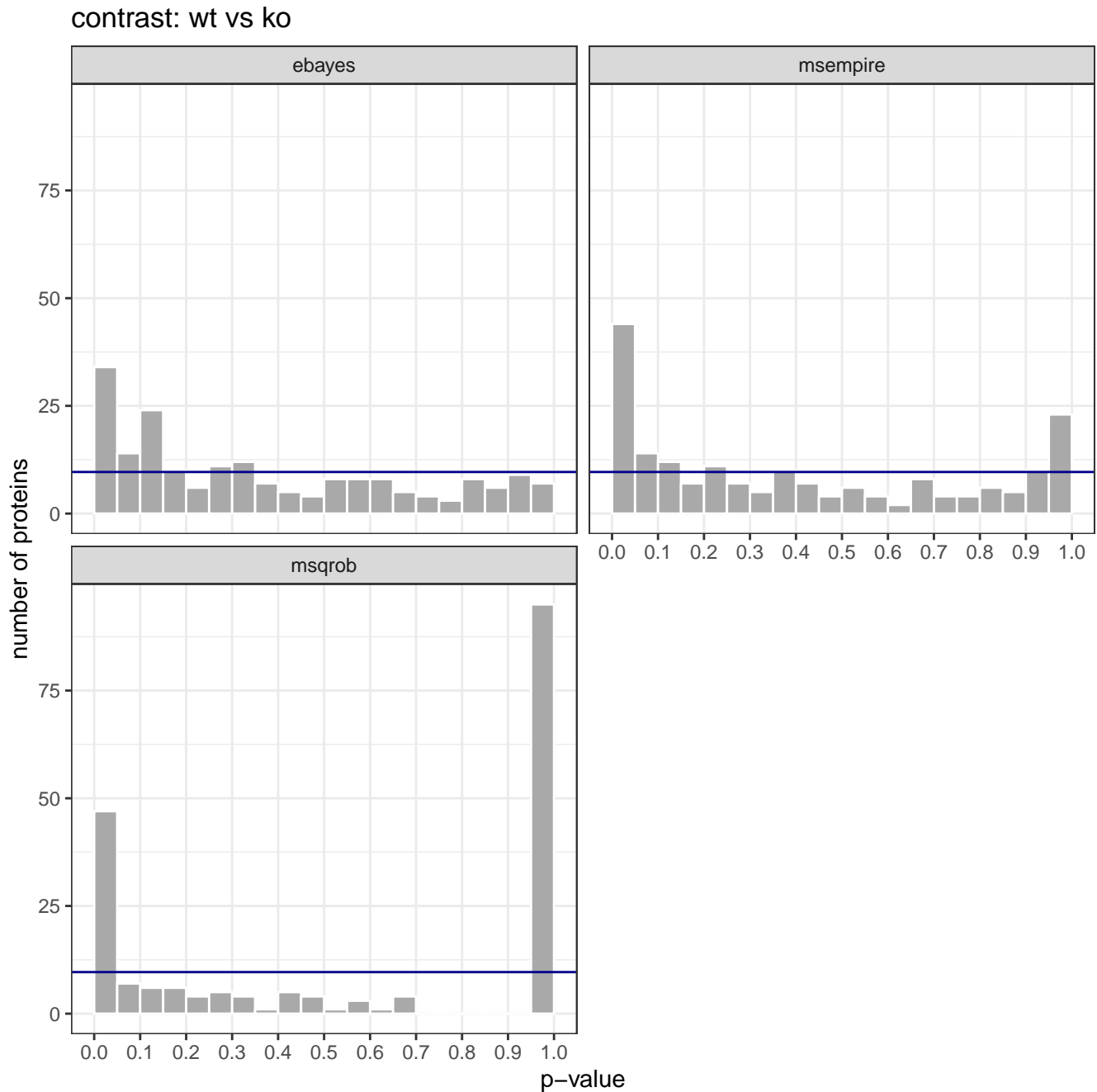
2.1.4 differential detect

Some proteins may not have peptides with sufficient abundance values for differential expression analysis, but do show strong differences in the number of detected peptides between sample groups. A simple z-score is computed for each protein based on the number of detected peptides per sample group. DEA is much more powerful for differential testing, but theze z-scores can offer complementary information in some experimental designs (e.g. a wildtype-knockout APMS study).

Below figure shows the distribution of these scores with thresholds at 2 std. Both the z-scores and the counts these are based upon are available in the statistical result Excel table.

contrast: wt vs ko

#proteins:541 #candidates:22
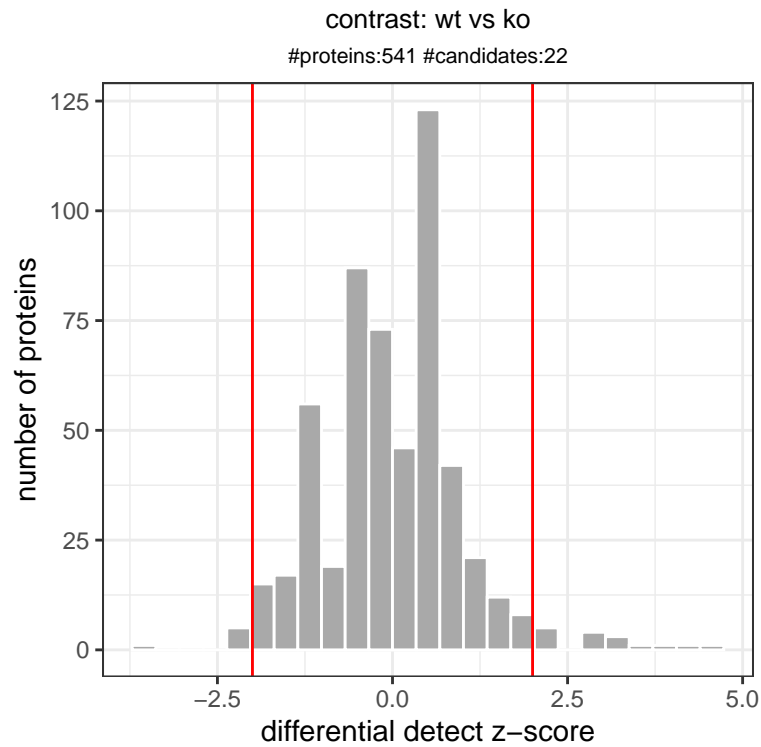
3 Summary of differential testing

Differential Expression Analysis: number of proteins found statistically significant.

contrast	algorithm	#test	#hits	top10 significant
wt vs ko	ebayes	193	4	camk2b, gpd2, ddx5, dnm1
wt vs ko	msempire	193	10	grid2, ddx5, ywhaq, camk2b, slc1a6, hk1, ap2b1, ywhae, snap25, igsf9b
wt vs ko	msqrob	193	10	grid2, camk2b, slc1a6, ddx5, ap2b1, tmem11, atp5j2, ywhaq, atp5i, llgl1

Differential Detection: prioritize proteins with more peptide detections in some group. A simple metric to complement results from DEA, which is the main result (eg; consider proteins with too few data points for DEA).

contrast	#test	#hits	top10 candidates
wt vs ko	541	22	gria2, shisa6, gria3, gria1, acap3, camk2g, camk2b, camk2a, nedd4l, camk2d

4 log

[info] reading MetaMorpheus search task...

[info] Parsing MetaMorpheus protein-groups, all non-unique peptides were assigned to their largest protein-group (by peptide count)

[info] 2850 target precursors, 2798 (plain)sequences, 682 proteins

[info] 1131/1131 protein accessions and 682/682 protein groups were mapped to provided fasta file(s)

[progress] filtered proteins: >tr|A0A075B5J6|A0A075B5J6__MOUSE Predicted gene, 20730 OS=Mus musculus OX=10090 GN=Gm20730 PE=4 SV=7;>sp|P01629|KV2A4__MOUS ... >tr|A0A075B5J9|A0A075B5J9__MOUSE Isoform of A0A0G2JDN5, Immunoglobulin kappa variable 17-127 OS=Mus musculus OX=10090 GN=I ... >tr|A0A075B5K0|A0A075B5K0__MOUSE Immunoglobulin kappa variable 14-126 (Fragment) OS=Mus musculus OX=10090 GN=Igkv14-126 PE ... >tr|A0A075B5K1|A0A075B5K1__MOUSE Isoform of P01650, Immunoglobulin kappa variable 11-125 OS=Mus musculus OX=10090 GN=Igkv1 ... >tr|A0A075B5K2|A0A075B5K2__MOUSE Isoform of A0A0G2JDR3, Immunoglobulin kappa chain variable 9-124 OS=Mus musculus OX=10090 ... >tr|A0A075B5K5|A0A075B5K5__MOUSE Isoform of P01627, Immunoglobulin kappa variable 2-112 OS=Mus musculus OX=10090 GN=Igkv2- ... >tr|A0A075B5K6|A0A075B5K6__MOUSE Immunoglobulin kappa variable 2-109 (Fragment) OS=Mus musculus OX=10090 GN=Igkv2-109 PE=4 ... >tr|A0A075B5K7|A0A075B5K7__MOUSE Isoform of A0A0G2JG36, Immunoglobulin kappa chain variable 14-100 OS=Mus musculus OX=1009 ... >tr|A0A075B5K9|A0A075B5K9__MOUSE Isoform of A0A0G2JGF9, Immunoglobulin kappa variable 12-98 OS=Mus musculus OX=10090 GN=Ig ... >tr|A0A075B5L1|A0A075B5L1__MOUSE Immunoglobulin kappa variable 10-94 (Fragment) OS=Mus musculus OX=10090 GN=Igkv10-94 PE=4 ... >tr|A0A075B5L7|A0A075B5L7__MOUSE Immunoglobulin kappa variable 4-80 (Fragment) OS=Mus musculus OX=10090 GN=Igkv4-80 PE=4 SV=2 >tr|A0A075B5M1|A0A075B5M1__MOUSE Isoform of A0A0G2JFU6, Immunoglobulin kappa variable 4-63 OS=Mus musculus OX=10090 GN=Igk ... >tr|A0A075B5M3|A0A075B5M3__MOUSE Isoform of A0A0G2JGI6, Immunoglobulin kappa variable 4-58 OS=Mus musculus OX=10090 GN=Igk ... >tr|A0A075B5M7|A0A075B5M7__MOUSE Isoform of A0A0G2JDV4, Immunoglobulin kappa variable 5-39 OS=Mus musculus OX=10090 GN=Igk ... >tr|A0A075B5N2|A0A075B5N2__MOUSE Isoform of A0A0G2JEI6, Immunoglobulin kappa chain variable 6-29 OS=Mus musculus OX=10090 ... >tr|A0A075B5N3|A0A075B5N3__MOUSE Isoform of A0A0G2JE47, Immunoglobulin kappa variable 8-28 OS=Mus musculus OX=10090 GN=Igk ... >tr|A0A075B5N4|A0A075B5N4__MOUSE Isoform of A0A0G2JF28, Immunoglobulin kappa chain variable 8-27 OS=Mus musculus OX=10090 ... >tr|A0A075B5N5|A0A075B5N5__MOUSE Immunoglobulin kappa variable 8-26 (Fragment) OS=Mus musculus OX=10090 GN=Igkv8-26 PE=4 SV=7 >tr|A0A075B5N6|A0A075B5N6__MOUSE Isoform of A0A0G2JDG9, Immunoglobulin kappa variable 8-16 OS=Mus musculus OX=10090 GN=Igk ... >tr|A0A075B5N7|A0A075B5N7__MOUSE Isoform of A0A0G2JGY3, Immunoglobulin kappa variable 6-13 OS=Mus musculus OX=10090 GN=Igk ... >tr|A0A075B5N9|A0A075B5N9__MOUSE Isoform of A0A0G2JE31, Immunoglobulin kappa variable 3-7 OS=Mus musculus OX=10090 GN=Igkv ... >tr|A0A075B5P1|A0A075B5P1__MOUSE Immunoglobulin kappa variable 3-1 (Fragment) OS=Mus musculus OX=10090 GN=Igkv3-1 PE=1 SV=7 >tr|A0A075B5P3|A0A075B5P3__MOUSE Isoform of P01867, Immunoglobulin heavy constant gamma 2B (Fragment) OS=Mus musculus OX=1 ... >tr|A0A075B5P4|A0A075B5P4__MOUSE Isoform of P01869, Ig gamma-1 chain C region secreted form (Fragment) OS=Mus musculus OX= ... >tr|A0A075B5P5|A0A075B5P5__MOUSE Isoform of A0A1Y7VJN6, Immunoglobulin heavy constant gamma 3 (Fragment) OS=Mus musculus O ... >tr|A0A075B5P9|A0A075B5P9__MOUSE Immunoglobulin heavy variable 5-4 (Fragment) OS=Mus musculus OX=10090 GN=Ighv5-4 PE=4 SV=1 >tr|A0A075B5Q2|A0A075B5Q2__MOUSE Immunoglobulin heavy variable 5-9 (Fragment) OS=Mus musculus OX=10090 GN=Ighv5-9 PE=4 SV=1 >tr|A0A075B5Q3|A0A075B5Q3__MOUSE Isoform of A0A0A6YY69, Immunoglobulin heavy variable 2-5 OS=Mus musculus OX=10090 GN=Ighv ... >tr|A0A075B5Q4|A0A075B5Q4__MOUSE Immunoglobulin heavy variable 5-12 (Fragment) OS=Mus musculus OX=10090 GN=Ighv5-12 PE=4 SV=1 >tr|A0A075B5Q6|A0A075B5Q6__MOUSE Isoform of A0A0A6YVS4, Immunoglobulin heavy variable 5-9-1 OS=Mus musculus OX=10090 GN=Ig ... >tr|A0A075B5Q9|A0A075B5Q9__MOUSE Isoform of A0A0A6YWC7, Immunoglobulin heavy variable 5-15 OS=Mus musculus OX=10090 GN=Igh ... >tr|A0A075B5R0|A0A075B5R0__MOUSE Isoform of A0A0B4J1P4, Immunoglobulin heavy variable 5-16 OS=Mus musculus OX=10090 GN=Igh ... >tr|A0A075B5R1|A0A075B5R1__MOUSE Immunoglobulin heavy variable 5-17 (Fragment) OS=Mus musculus OX=10090 GN=Ighv5-17 PE=4 SV=1 >tr|A0A075B5R2|A0A075B5R2__MOUSE Immunoglobulin heavy variable 7-3 (Fragment) OS=Mus musculus OX=10090 GN=Ighv7-3 PE=4 SV=2 >tr|A0A075B5R4|A0A075B5R4__MOUSE Immunoglobulin heavy variable 14-1 (Fragment) OS=Mus musculus OX=10090 GN=Ighv14-1 PE=4 SV=1 >tr|A0A075B5R5|A0A075B5R5__MOUSE Immunoglobulin heavy variable 4-1 (Fragment) OS=Mus musculus OX=10090 GN=Ighv4-1 PE=1 SV=7 >tr|A0A075B5R7|A0A075B5R7__MOUSE Immunoglobulin heavy variable 14-2 (Fragment) OS=Mus musculus OX=10090 GN=Ighv14-2 PE=4 SV=1 >tr|A0A075B5S2|A0A075B5S2__MOUSE Immunoglobulin heavy variable 7-1 (Fragment) OS=Mus musculus OX=10090 GN=Ighv7-1 PE=1 SV=2 >tr|A0A075B5S5|A0A075B5S5__MOUSE Isoform of A0A0A6YXL5, Immunoglobulin heavy variable 7-4 OS=Mus musculus OX=10090 GN=Ighv ... >tr|A0A075B5S9|A0A075B5S9__MOUSE Isoform of A0A0A6YWH6, Immunoglobulin heavy variable 9-4 OS=Mus musculus OX=10090 GN=Ighv ... >tr|A0A075B5T2|A0A075B5T2__MOUSE Immunoglobulin heavy variable 6-3 (Fragment) OS=Mus musculus OX=10090 GN=Ighv6-3 PE=4 SV=7 >tr|A0A075B5T3|A0A075B5T3__MOUSE Immunoglobulin heavy variable 6-6 (Fragment) OS=Mus musculus OX=10090 GN=Ighv6-6 PE=4 SV=1 >tr|A0A075B5T4|A0A075B5T4__MOUSE Immunoglobulin heavy variable 1-4 (Fragment) OS=Mus musculus OX=10090 GN=Ighv1-4 PE=4 SV=1 >tr|A0A075B5T5|A0A075B5T5__MOUSE Isoform of A0A0A6YWG2, Immunoglobulin heavy variable V1-5 OS=Mus musculus OX=10090 GN=Igh ... >tr|A0A075B5T6|A0A075B5T6__MOUSE Immunoglobulin heavy variable V10-3 (Fragment) OS=Mus musculus OX=10090 GN=Ighv10-3 PE=4 SV=1 >tr|A0A075B5T9|A0A075B5T9__MOUSE Isoform of A0A0A6YW37, Immunoglobulin heavy variable V1-9 OS=Mus musculus OX=10090 GN=Igh ... >tr|A0A075B5U6|A0A075B5U6__MOUSE Isoform of A0A0A6YX66, Immunoglobulin heavy variable V1-20 OS=Mus musculus OX=10090 GN=Ig ... >tr|A0A075B5U7|A0A075B5U7__MOUSE Immunoglobulin heavy variable 1-22 (Fragment) OS=Mus musculus OX=10090 GN=Ighv1-22 PE=1 SV=1 >tr|A0A075B5V5|A0A075B5V5__MOUSE Immunoglobulin heavy variable 1-39 (Fragment) OS=Mus musculus OX=10090 GN=Ighv1-39 PE=4 SV=1 >tr|A0A075B5V6|A0A075B5V6__MOUSE Isoform of A0A0A6YY38, Immunoglobulin heavy variable V1-42 OS=Mus musculus OX=10090 GN=Ig ... >tr|A0A075B5V7|A0A075B5V7__MOUSE Isoform of A0A0A6YXN5, Immunoglobulin heavy variable V1-43 OS=Mus musculus OX=10090 GN=Ig ... >tr|A0A075B5V8|A0A075B5V8__MOUSE Isoform of A0A0A6YY41, Immunoglobulin heavy variable 1-47 OS=Mus musculus OX=10090 GN=Igh ... >tr|A0A075B5W2|A0A075B5W2__MOUSE Isoform of A0A0A6YXC3, Immunoglobulin heavy variable 1-52 OS=Mus musculus OX=10090 GN=Igh ... >tr|A0A075B5W3|A0A075B5W3__MOUSE Immunoglobulin heavy variable 1-53 (Fragment) OS=Mus musculus OX=10090 GN=Ighv1-53 PE=4 SV=1 >tr|A0A075B5W4|A0A075B5W4__MOUSE Isoform of A0A0A6YXA3, Immunoglobulin heavy variable V8-6 OS=Mus musculus OX=10090 GN=Igh ... >tr|A0A075B5W5|A0A075B5W5__MOUSE Immunoglobulin heavy variable V1-54 (Fragment) OS=Mus musculus OX=10090 GN=Ighv1-54 PE=4 SV=1 >tr|A0A075B5W6|A0A075B5W6__MOUSE Immunoglobulin heavy variable 1-55 (Fragment) OS=Mus musculus OX=10090 GN=Ighv1-55 PE=1 SV=1 >tr|A0A075B5W9|A0A075B5W9__MOUSE Immunoglobulin heavy variable 1-58 (Fragment) OS=Mus musculus OX=10090 GN=Ighv1-58 PE=4 SV=1 >tr|A0A075B5X3|A0A075B5X3__MOUSE Immunoglobulin heavy variable 1-64 (Fragment) OS=Mus musculus OX=10090 GN=Ighv1-64 PE=4 SV=1 >tr|A0A075B5X7|A0A075B5X7__MOUSE Isoform of A0A0G2JFS5, Immunoglobulin heavy variable 1-69 OS=Mus musculus OX=10090 GN=Igh ... >tr|A0A075B5Y1|A0A075B5Y1__MOUSE Isoform of A0A0G2JGK2, Immunoglobulin heavy variable V1-74 OS=Mus musculus OX=10090 GN=Ig ... >tr|A0A075B5Y2|A0A075B5Y2__MOUSE Immunoglobulin heavy variable 1-75 (Fragment) OS=Mus musculus OX=10090 GN=Ighv1-75 PE=4 SV=1 >tr|A0A075B5Y3|A0A075B5Y3__MOUSE Immunoglobulin heavy variable 1-80 (Fragment) OS=Mus musculus OX=10090 GN=Ighv1-80 PE=1 SV=1 >tr|A0A075B5Y4|A0A075B5Y4__MOUSE Immunoglobulin heavy variable 1-81 (Fragment) OS=Mus musculus OX=10090 GN=Ighv1-81 PE=4 SV=1 >tr|A0A075B5Y5|A0A075B5Y5__MOUSE Isoform of P06327, Immunoglobulin heavy variable 1-84 (Fragment) OS=Mus musculus OX=10090 ... >tr|A0A075B5Y6|A0A075B5Y6__MOUSE

Immunoglobulin heavy variable 1-85 (Fragment) OS=Mus musculus OX=10090 GN=Ighv1-85 PE=4 SV=1 >tr|A0A075B666|A0A075B666__MOUSE
Immunoglobulin kappa chain variable 13-85 (Fragment) OS=Mus musculus OX=10090 GN=Igkv13-8 . . . >tr|A0A075B674|A0A075B674__MOUSE
Isoform of A0A0G2JGN3, Immunoglobulin heavy variable 1-78 OS=Mus musculus OX=10090 GN=Igh . . . >tr|A0A075B677|A0A075B677__MOUSE
Isoform of A0A0G2JFC6, Immunoglobulin kappa variable 4-53 OS=Mus musculus OX=10090 GN=Igk . . . >tr|A0A075B680|A0A075B680__MOUSE
Isoform of A0A0A6YXZ4, Immunoglobulin heavy variable 1-62-2 OS=Mus musculus OX=10090 GN=I . . . >tr|A0A075B684|A0A075B684__MOUSE
Isoform of A0A075B5U3, Immunoglobulin heavy variable 1-62-1 OS=Mus musculus OX=10090 GN=I . . . >tr|A0A075B696|A0A075B696__MOUSE
Immunoglobulin heavy variable 2-3 (Fragment) OS=Mus musculus OX=10090 GN=Ighv2-3 PE=4 SV=3 >tr|A0A075B6D5|A0A075B6D5__MOUSE
Isoform of A0A0G2JFZ3, Immunoglobulin kappa chain variable 19-93 OS=Mus musculus OX=10090 . . . >tr|A0A087WPN7|A0A087WPN7__MOUSE
Isoform of A0A0A6YWN3, Immunoglobulin heavy variable 13-2 OS=Mus musculus OX=10090 GN=Igh . . . >tr|A0A0A0MQC1|A0A0A0MQC1__MOUSE
Isoform of P18533, Immunoglobulin heavy variable 3-5 OS=Mus musculus OX=10090 GN=Ighv3-5 . . . >tr|A0A0A6YVW3|A0A0A6YVW3__MOUSE
Immunoglobulin heavy variable V1-23 (Fragment) OS=Mus musculus OX=10090 GN=Ighv1-23 PE=4 . . . >tr|A0A0A6YWI9|A0A0A6YWI9__MOUSE
Immunoglobulin heavy variable V1-11 (Fragment) OS=Mus musculus OX=10090 GN=Ighv1-11 PE=4 SV=1 >tr|A0A0A6YXN4|A0A0A6YXN4__MOUSE
Immunoglobulin heavy variable V1-18 (Fragment) OS=Mus musculus OX=10090 GN=Ighv1-18 PE=1 SV=1 >tr|A0A0A6YXQ0|A0A0A6YXQ0__MOUSE
Immunoglobulin heavy variable 8-8 (Fragment) OS=Mus musculus OX=10090 GN=Ighv8-8 PE=4 SV=1 >tr|A0A0A6YY53|A0A0A6YY53__MOUSE
Isoform of F6TQW2, Immunoglobulin heavy constant gamma 2C (Fragment) OS=Mus musculus OX=1 . . . >tr|A0A0A6YYE7|A0A0A6YYE7__MOUSE
Immunoglobulin kappa variable 4-57 (Fragment) OS=Mus musculus OX=10090 GN=Igkv4-57 PE=4 SV=2 >tr|A0A0B4J1H6|A0A0B4J1H6__MOUSE
Immunoglobulin kappa chain variable 2-137 (Fragment) OS=Mus musculus OX=10090 GN=Igkv2-13 . . . >tr|A0A0B4J1H7|A0A0B4J1H7__MOUSE
Immunoglobulin kappa variable 1-135 (Fragment) OS=Mus musculus OX=10090 GN=Igkv1-135 PE=4 . . . >tr|A0A0B4J1H9|A0A0B4J1H9__MOUSE
Immunoglobulin kappa variable 1-132 (Fragment) OS=Mus musculus OX=10090 GN=Igkv1-132 PE=4 . . . >tr|A0A0B4J1I1|A0A0B4J1I1__MOUSE
Immunoglobulin kappa variable 16-104 (Fragment) OS=Mus musculus OX=10090 GN=Igkv16-104 PE . . . >tr|A0A0B4J1I4|A0A0B4J1I4__MOUSE
Immunoglobulin kappa chain variable 4-72 (Fragment) OS=Mus musculus OX=10090 GN=Igkv4-72 . . . >tr|A0A0B4J1I7|A0A0B4J1I7__MOUSE
Immunoglobulin kappa variable 4-68 (Fragment) OS=Mus musculus OX=10090 GN=Igkv4-68 PE=4 SV=1 >tr|A0A0B4J1I8|A0A0B4J1I8__MOUSE
Immunoglobulin kappa variable 4-59 (Fragment) OS=Mus musculus OX=10090 GN=Igkv4-59 PE=4 S . . . >tr|A0A0B4J1I9|A0A0B4J1I9__MOUSE
Isoform of P04945, Immunoglobulin kappa variable 4-55 (Fragment) OS=Mus musculus OX=10090 . . . >tr|A0A0B4J1J0|A0A0B4J1J0__MOUSE
Immunoglobulin kappa variable 4-50 (Fragment) OS=Mus musculus OX=10090 GN=Igkv4-50 PE=4 SV=1 >tr|A0A0B4J1J2|A0A0B4J1J2__MOUSE
Immunoglobulin kappa chain variable 5-43 (Fragment) OS=Mus musculus OX=10090 GN=Igkv5-43 . . . >tr|A0A0B4J1J4|A0A0B4J1J4__MOUSE
Immunoglobulin heavy variable V9-2 (Fragment) OS=Mus musculus OX=10090 GN=Ighv9-2 PE=4 SV=1 >tr|A0A0B4J1J5|A0A0B4J1J5__MOUSE
Immunoglobulin heavy variable V9-3 (Fragment) OS=Mus musculus OX=10090 GN=Ighv9-3 PE=1 SV=1 >tr|A0A0B4J1J6|A0A0B4J1J6__MOUSE
Immunoglobulin heavy variable 10-1 (Fragment) OS=Mus musculus OX=10090 GN=Ighv10-1 PE=4 SV=1 >tr|A0A0B4J1J7|A0A0B4J1J7__MOUSE
Isoform of A0A0G2JEU7, Immunoglobulin heavy variable 1-82 OS=Mus musculus OX=10090 GN=Igh . . . >tr|A0A0B4J1M0|A0A0B4J1M0__MOUSE
Isoform of A0A0G2JGS9, Immunoglobulin heavy variable 1-77 OS=Mus musculus OX=10090 GN=Igh . . . >tr|A0A0B4J1N0|A0A0B4J1N0__MOUSE
Isoform of A0A0G2JFE9, Immunoglobulin heavy variable 1-76 OS=Mus musculus OX=10090 GN=Igh . . . >tr|A0A0G2JDE1|A0A0G2JDE1__MOUSE
Immunoglobulin heavy variable V8-12 (Fragment) OS=Mus musculus OX=10090 GN=Ighv8-12 PE=1 SV=1 >tr|A0A0G2JE99|A0A0G2JE99__MOUSE
Immunoglobulin lambda constant 1 (Fragment) OS=Mus musculus OX=10090 GN=Iglc1 PE=4 SV=1;> . . . >tr|A0A0G2JGQ8|A0A0G2JGQ8__MOUSE
Isoform of P01845, Ig lambda-3 chain C region (Fragment) OS=Mus musculus OX=10090 GN=Iglc . . . >tr|A0A140T8M0|A0A140T8M0__MOUSE
Immunoglobulin kappa variable 1-117 (Fragment) OS=Mus musculus OX=10090 GN=Igkv1-117 PE=4 . . . >tr|A0A140T8M2|A0A140T8M2__MOUSE
Immunoglobulin kappa variable 12-44 (Fragment) OS=Mus musculus OX=10090 GN=Igkv12-44 PE=4 . . . >tr|A0A140T8M3|A0A140T8M3__MOUSE
Immunoglobulin kappa chain variable 8-30 (Fragment) OS=Mus musculus OX=10090 GN=Igkv8-30 . . . >tr|A0A140T8M4|A0A140T8M4__MOUSE
Isoform of A0A0G2JFN8, Immunoglobulin kappa variable 8-19 OS=Mus musculus OX=10090 GN=Igk . . . >tr|A0A140T8M5|A0A140T8M5__MOUSE
Immunoglobulin kappa variable 6-15 (Fragment) OS=Mus musculus OX=10090 GN=Igkv6-15 PE=1 SV=2 >tr|A0A140T8N0|A0A140T8N0__MOUSE
Isoform of P01639, Immunoglobulin kappa chain variable 9-120 (Fragment) OS=Mus musculus O . . . >tr|A0A140T8N2|A0A140T8N2__MOUSE
Isoform of P01642, Protein Igkv5-48 (Fragment) OS=Mus musculus OX=10090 GN=Igkv5-48 PE=1 . . . >tr|A0A140T8N3|A0A140T8N3__MOUSE
Immunoglobulin kappa chain variable 13-84 (Fragment) OS=Mus musculus OX=10090 GN=Igkv13-8 . . . >tr|A0A140T8N5|A0A140T8N5__MOUSE
Immunoglobulin kappa variable 6-23 (Fragment) OS=Mus musculus OX=10090 GN=Igkv6-23 PE=4 SV=2 >tr|A0A140T8N7|A0A140T8N7__MOUSE
Immunoglobulin kappa chain variable 6-25 (Fragment) OS=Mus musculus OX=10090 GN=Igkv6-25 . . . >tr|A0A140T8N8|A0A140T8N8__MOUSE
Immunoglobulin kappa variable 9-123 (Fragment) OS=Mus musculus OX=10090 GN=Igkv9-123 PE=4 . . . >tr|A0A140T8N9|A0A140T8N9__MOUSE
Immunoglobulin kappa variable 6-32 (Fragment) OS=Mus musculus OX=10090 GN=Igkv6-32 PE=4 SV=2 >tr|A0A140T8P1|A0A140T8P1__MOUSE
Immunoglobulin kappa variable 6-14 (Fragment) OS=Mus musculus OX=10090 GN=Igkv6-14 PE=4 SV=2 >tr|A0A140T8P3|A0A140T8P3__MOUSE
Immunoglobulin kappa chain variable 15-103 (Fragment) OS=Mus musculus OX=10090 GN=Igkv15- . . . >tr|A0A140T8P5|A0A140T8P5__MOUSE
Immunoglobulin kappa chain variable 8-24 (Fragment) OS=Mus musculus OX=10090 GN=Igkv8-24 . . . >tr|A0A140T8P6|A0A140T8P6__MOUSE
Immunoglobulin kappa variable 12-46 (Fragment) OS=Mus musculus OX=10090 GN=Igkv12-46 PE=1 . . . >tr|A0A140T8P7|A0A140T8P7__MOUSE
Immunoglobulin kappa variable 8-21 (Fragment) OS=Mus musculus OX=10090 GN=Igkv8-21 PE=1 SV=2 >tr|A0A140T8P9|A0A140T8P9__MOUSE
Immunoglobulin kappa variable 14-111 (Fragment) OS=Mus musculus OX=10090 GN=Igkv14-111 PE . . . >tr|A0A140T8Q1|A0A140T8Q1__MOUSE
Isoform of P01635, Protein Igkv12-41 (Fragment) OS=Mus musculus OX=10090 GN=Igkv12-41 PE= . . . >sp|P01631|KV2A7__MOUSE Ig kappa chain V-II region 26-10 OS=Mus musculus OX=10090 PE=1 SV=1 >sp|P01633|KV5A1__MOUSE Ig kappa chain V19-17 OS=Mus musculus OX=10090 GN=Igk-V19-17 PE=1 SV=1 >sp|P01636|KV5A4__MOUSE Ig kappa chain V-V region MOPC 149 OS=Mus musculus OX=10090 PE=1 SV=1 >sp|P01644|KV5AB__MOUSE Ig kappa chain V-V region HP R16.7 OS=Mus musculus OX=10090 PE=1 SV=1;>sp|P01645|KV5AC__MOUSE Ig ka . . . >sp|P01654|KV3A1__MOUSE Ig kappa chain V-III region PC 2880/PC 1229 OS=Mus musculus OX=10090 PE=1 SV=1 >sp|P01660|KV3A8__MOUSE Ig kappa chain V-III region PC 3741/TEPC 111 OS=Mus musculus OX=10090 PE=1 SV=1 >sp|P01665|KV3AD__MOUSE Ig kappa chain V-III region PC 7043 OS=Mus musculus OX=10090 PE=1 SV=1;>sp|P01666|KV3AE__MOUSE Ig k . . . >sp|P01671|KV3AJ__MOUSE Ig kappa chain V-III region PC 7175 OS=Mus musculus OX=10090 PE=1 SV=1 >sp|P01675|KV6A1__MOUSE Ig kappa chain V-VI region XRPC 44 OS=Mus musculus OX=10090 PE=1 SV=1;>sp|P01676|KV6A2__MOUSE Ig ka . . . >sp|P01837|IGKC__MOUSE Immunoglobulin kappa constant OS=Mus musculus OX=10090 GN=Igkc PE=1 SV=2 >sp|P01844|LAC2__MOUSE Ig lambda-2 chain C region OS=Mus musculus OX=10090 GN=Iglc2 PE=1 SV=1;>tr|Q99JC1|Q99JC1__MOUSE Isof . . . >sp|P01863|GCAA__MOUSE Ig gamma-2A chain C region, A allele OS=Mus musculus OX=10090 GN=Ighg PE=1 SV=1;>sp|P01865|GCAM__MOU . . . >sp|P01864|GCAB__MOUSE Ig gamma-2A chain C region secreted form OS=Mus musculus OX=10090 PE=1 SV=1 >sp|P03977|KV3A4__MOUSE Ig kappa chain V-III region 50S10.1 OS=Mus musculus OX=10090 PE=1 SV=1 >sp|P06330|HVM51__MOUSE Ig heavy chain V region AC38 205.12 OS=Mus musculus OX=10090 PE=1 SV=1 >sp|P18528|HVM57__MOUSE Ig heavy chain V region 6.96 OS=Mus musculus OX=10090 PE=4 SV=1 >sp|P18529|HVM58__MOUSE Ig heavy chain V region 5-76 OS=Mus musculus OX=10090 PE=1 SV=1 >sp|P18531|HVM60__MOUSE Ig heavy chain V region 3-6 OS=Mus musculus OX=10090 GN=Ighv3-6 PE=1 SV=1 >sp|P84750|KVM5__MOUSE Ig kappa chain V region Mem5 (Fragment) OS=Mus musculus OX=10090 PE=1 SV=1 >sp|Q3UV17|K22O__MOUSE Keratin, type II cytoskeletal 2 oral OS=Mus musculus OX=10090 GN=Krt76 PE=1 SV=1 >tr|Q792Z1|Q792Z1__MOUSE MCG140784 OS=Mus musculus OX=10090 GN=Try10 PE=1 SV=1 >sp|Q9Z320|K1C27__MOUSE Keratin, type I cytoskeletal 27 OS=Mus musculus OX=10090 GN=Krt27 PE=1 SV=1

[info] 141/682 proteins matching your filters were removed from the dataset

[info] contrast: wt vs ko

[info] sample metadata contains samples with multiple fractions, 'sample_id' with the same 'shortname' are now merged by summation of their respective peptide intensities

[info] using 7 threads for multiprocessing

[progress] caching filter data took 1 seconds

[progress] peptide filtering and normalization took 2 seconds

[info] differential abundance analysis for contrast: wt vs ko

[info] using data from peptide filter: global data filter

[info] log2 foldchange threshold estimated by bootstrap analysis: 0.965

[progress] eBayes took 1 seconds

[progress] MS-EmpiRe took 3 seconds

[progress] MSqRob took 12 seconds

[progress] creating PDF report. . .

[progress] report: constructing plots specific for each contrast

[progress] report: rendering report (this may take a while depending on dataset size)

[progress] RT plots: preparing data took 1 seconds

[progress] RT plots: creating plots took 1 seconds

5 R command history

This shows the history commands from your R script that starts this pipeline, thereby automatically documenting the parameters/settings used. All lines of executed code since (last) importing data using this R package are shown.

Using this feature

Do not use RStudio's `source` option to execute our pipeline since it will only write `source(...yourscript.R)` to the session history, and consequentially that is all you see in this 'code log'. Instead, select all lines in your script (`control + A`) and then "run" the selected code (either click the run button in RStudio, or use `control + enter`). All lines shown in this section are the same as shown in the RStudio 'History' pane (a tab on the top-right of its UI).

```r
dataset = import_dataset_metamorpheus(
  path = getwd(),
  protein_qval_threshold = 0.05
)
dataset = import_fasta(dataset,
  files = c(
    "UP000000589_10090.fasta",
    "UP000000589_10090_additional.fasta"
  )
)
dataset = remove_proteins_by_name(dataset,
  regular_expression = "ig \\S+ chain|keratin|GN=(krt|try|igk|igg|igkv|ighv|ighg)"
)
dataset = import_sample_metadata(dataset,
  filename = "sample_metadata.xlsx"
)
dataset = setup_contrasts(dataset,
  contrast_list = list(c(
    "wt",
    "ko"
  ))
)
dataset = analysis_quickstart(dataset,
  filter_min_detect = 1,
  filter_min_quant = 3,
  filter_by_contrast = FALSE,
  norm_algorithm = "msempire",
  dea_algorithm = c(
    "ebayes",
    "msempire", "msqrob"
  ),
  dea_qvalue_threshold = 0.05,
  dea_log2foldchange_threshold = NA,
  output_qc_report = TRUE,
  output_dir = getwd(),
  output_within_timestamped_subdirectory = TRUE
)
```

6 R session info

The computer system and versioning of all R packages used to run this analysis are shown below to facilitate, in combination with the previous section, reproducibility.

setting	value
version	R version 3.6.1 (2019-07-05)
os	Windows 10 x64
system	x86_64, mingw32
ui	RStudio
language	(EN)
collate	English_United States.1252
ctype	English_United States.1252
tz	Europe/Berlin
date	2020-06-11

System

package	loadedversion	source
dplyr	1.0.0	CRAN (R 3.6.3)
ggplot2	3.2.1	CRAN (R 3.6.1)
msdap	0.2.1	
rlang	0.4.6	CRAN (R 3.6.3)
testthat	2.3.2	CRAN (R 3.6.3)
tibble	2.1.3	CRAN (R 3.6.1)
tidyr	1.0.2	CRAN (R 3.6.2)

Attached packages

package	loadedversion	source
affy	1.64.0	Bioconductor
affyio	1.56.0	Bioconductor
askpass	1.1	CRAN (R 3.6.1)
assertthat	0.2.1	CRAN (R 3.6.1)
backports	1.1.5	CRAN (R 3.6.1)
Biobase	2.46.0	Bioconductor
BiocGenerics	0.32.0	Bioconductor
BiocManager	1.30.10	CRAN (R 3.6.3)
BiocParallel	1.20.1	Bioconductor
bit	1.1-14	CRAN (R 3.6.0)
bit64	0.9-7	CRAN (R 3.6.0)
boot	1.3-24	CRAN (R 3.6.2)
callr	3.4.3	CRAN (R 3.6.3)
cli	2.0.2	CRAN (R 3.6.3)
codetools	0.2-16	CRAN (R 3.6.1)
colorspace	1.4-1	CRAN (R 3.6.1)
cowplot	1.0.0	CRAN (R 3.6.1)
crayon	1.3.4	CRAN (R 3.6.1)
data.table	1.12.8	CRAN (R 3.6.2)
desc	1.2.0	CRAN (R 3.6.1)
devtools	2.3.0	CRAN (R 3.6.3)
digest	0.6.25	CRAN (R 3.6.1)
doParallel	1.0.15	CRAN (R 3.6.1)
ellipsis	0.3.0	CRAN (R 3.6.1)
evaluate	0.14	CRAN (R 3.6.1)
fansi	0.4.1	CRAN (R 3.6.2)
farver	2.0.3	CRAN (R 3.6.2)
fastmap	1.0.1	CRAN (R 3.6.1)
forcats	0.4.0	CRAN (R 3.6.1)
foreach	1.4.8	CRAN (R 3.6.2)
formatR	1.7	CRAN (R 3.6.1)
fs	1.3.1	CRAN (R 3.6.1)
generics	0.0.2	CRAN (R 3.6.1)
ggpubr	0.2.5	CRAN (R 3.6.2)
ggrepel	0.8.1	CRAN (R 3.6.1)
ggsignif	0.6.0	CRAN (R 3.6.1)
glue	1.4.1	CRAN (R 3.6.3)
gridExtra	2.3	CRAN (R 3.6.1)
gtable	0.3.0	CRAN (R 3.6.1)
gtools	3.8.1	CRAN (R 3.6.0)
hms	0.5.3	CRAN (R 3.6.2)
htmltools	0.4.0	CRAN (R 3.6.1)
htmlwidgets	1.5.1	CRAN (R 3.6.1)
httpuv	1.5.2	CRAN (R 3.6.1)
impute	1.60.0	Bioconductor
IRanges	2.20.2	Bioconductor
iterators	1.0.12	CRAN (R 3.6.1)
jsonlite	1.6.1	CRAN (R 3.6.2)
knitr	1.28	CRAN (R 3.6.2)
labeling	0.3	CRAN (R 3.6.0)

package	loadedversion	source
later	1.0.0	CRAN (R 3.6.1)
lattice	0.20-40	CRAN (R 3.6.1)
lazyeval	0.2.2	CRAN (R 3.6.1)
learnr	0.10.1	CRAN (R 3.6.3)
lifecycle	0.2.0	CRAN (R 3.6.3)
limma	3.42.2	Bioconductor
lme4	1.1-21	CRAN (R 3.6.1)
magrittr	1.5	CRAN (R 3.6.1)
MALDIquant	1.19.3	CRAN (R 3.6.1)
markdown	1.1	CRAN (R 3.6.1)
MASS	7.3-51.5	CRAN (R 3.6.2)
Matrix	1.2-18	CRAN (R 3.6.2)
matrixStats	0.55.0	CRAN (R 3.6.1)
memoise	1.1.0	CRAN (R 3.6.1)
mime	0.9	CRAN (R 3.6.2)
minqa	1.2.4	CRAN (R 3.6.1)
msEmpiRe	0.1.0	Github (zimmerlab/MS-EmpiRe@ae985a9)
MSnbase	2.12.0	Bioconductor
munsell	0.5.0	CRAN (R 3.6.1)
mzID	1.24.0	Bioconductor
mzR	2.20.0	Bioconductor
ncdf4	1.17	CRAN (R 3.6.1)
nlme	3.1-144	CRAN (R 3.6.2)
nloptr	1.2.1	CRAN (R 3.6.1)
openxlsx	4.1.4	CRAN (R 3.6.2)
packrat	0.5.0	CRAN (R 3.6.3)
patchwork	1.0.0	CRAN (R 3.6.3)
pcaMethods	1.78.0	Bioconductor
pdftools	2.3	CRAN (R 3.6.1)
pillar	1.4.3	CRAN (R 3.6.2)
pkgbuild	1.0.6	CRAN (R 3.6.1)
pkgconfig	2.0.3	CRAN (R 3.6.1)
pkgload	1.0.2	CRAN (R 3.6.1)
plyr	1.8.5	CRAN (R 3.6.2)
preprocessCore	1.48.0	Bioconductor
prettyunits	1.1.1	CRAN (R 3.6.2)
pROC	1.16.1	CRAN (R 3.6.2)
processx	3.4.2	CRAN (R 3.6.2)
promises	1.1.0	CRAN (R 3.6.1)
ProtGenerics	1.18.0	Bioconductor
ps	1.3.2	CRAN (R 3.6.2)
purrr	0.3.3	CRAN (R 3.6.1)
qpdf	1.1	CRAN (R 3.6.1)
R6	2.4.1	CRAN (R 3.6.1)
RColorBrewer	1.1-2	CRAN (R 3.6.0)
Rcpp	1.0.3	CRAN (R 3.6.1)
readr	1.3.1	CRAN (R 3.6.1)
remotes	2.1.1	CRAN (R 3.6.2)
reshape2	1.4.3	CRAN (R 3.6.1)
rmarkdown	2.1	CRAN (R 3.6.2)

package	loadedversion	source
rprojroot	1.3-2	CRAN (R 3.6.1)
rstudioapi	0.11	CRAN (R 3.6.2)
S4Vectors	0.24.3	Bioconductor
scales	1.1.0	CRAN (R 3.6.1)
sessioninfo	1.1.1	CRAN (R 3.6.1)
shiny	1.4.0	CRAN (R 3.6.1)
shinyFiles	0.8.0	CRAN (R 3.6.3)
shinyjs	1.1	CRAN (R 3.6.2)
sortable	0.4.2	CRAN (R 3.6.3)
stringi	1.4.6	CRAN (R 3.6.2)
stringr	1.4.0	CRAN (R 3.6.1)
styler	1.3.2	CRAN (R 3.6.2)
tidyselect	1.1.0	CRAN (R 3.6.3)
tinytex	0.20	CRAN (R 3.6.2)
usethis	1.6.1	CRAN (R 3.6.3)
utf8	1.1.4	CRAN (R 3.6.1)
vctrs	0.3.1	CRAN (R 3.6.3)
viridis	0.5.1	CRAN (R 3.6.1)
viridisLite	0.3.0	CRAN (R 3.6.1)
vsn	3.54.0	Bioconductor
withr	2.1.2	CRAN (R 3.6.1)
xfun	0.12	CRAN (R 3.6.2)
XML	3.98-1.20	CRAN (R 3.6.0)
xtable	1.8-4	CRAN (R 3.6.1)
yaml	2.2.1	CRAN (R 3.6.2)
zip	2.0.4	CRAN (R 3.6.1)
zlibbioc	1.32.0	Bioconductor

Packages that are not attached