

 represents actual function name

Explanatory data analysis: (Pre-analysis)

Data Process

dataProcess

- Data format: long format(Skyline, MultiQuant)
- Summary report: feature, sample, missingness(warning messages)
- Logarithm transformation with base 2 or 10
- Normalization: bias of MS run

Visualization

dataProcessPlots

- Profile plot
- Quality control plot
- Condition plot

Model-based analysis: (testing)

Comparisons between conditions

groupComparison

- lists of adjusted p-values fitted with a variety of models
 - label-based or label-free
 - expanded or restricted scope of Biological or Technical replication
 - Account interference transition or not
 - Account unequal variance among features
 - Multiple comparisons

Visualization

modelBasedQCPlots

- Residual plot
- Normal quantile-quantile plot

Visualization

groupComparisonPlots

- Heatmap
- Volcano plot
- Comparison plot

Design for future experiments

Sample size calculation

designSampleSize

- Sample size calculation: # of biological replicates, peptides, transition; according to FDR and CV
- Power calculation

Visualization

designSampleSizePlots

Model-based quantification

Quantification

quantification

- Sample quantification
- Group quantification