

Workflow for analysis of raw data

Functions with their main arguments (see help pages for a complete description)

Step 1: import, check and pretreatment

```
microarraydata(file,
    norm.method = c("cyclicloess", "quantile", "scale", "none"))
RNAseqdata(file, transfo.method = c("rlog", "vst"))
continuousomicdata(file)
continuousanchoringdata(file)
```

Step 2: selection of significantly responsive items

```
itemselect(omicdata,
    select.method = c("quadratic", "linear", "ANOVA"), FDR)
```

Step 3: dose-response modelling for responsive items

drcfit(itemselect, information.criterion = c("AICc", "BIC", "AIC"))

Step 4: Computation of benchmark doses

bmdcalc(f, z = 1, x = 10, minBMD)

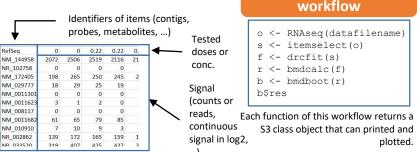
Step 5: Bootstrap to compute BMD confidence intervals

bmdboot(r, niter = 1000, conf.level = 0.95)

Format of data in input

Data can be imported from a .txt file (e.g. "mydata.txt") containing one row per item after a first row giving the doses or concentrations for each sample , with the first column corresponding to the identifier of each item. Alternatively an R object of class data.frame can be directly given in input, corresponding to the output of read.table(file, header = FALSE) on a file described as above.

Typical script for the workflow



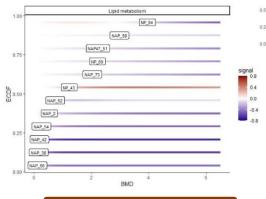
Other functions to help the interpretation of results winthin a multi-omics approach using a same biological annotation

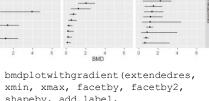
Functions taking as a first argument extendedres, a dataframe with the main workflow results, extended with additional columns coding for example for a biological of items. Some lines of the workflow results can be replicated for items having more than one annotation. Results obtained on different molecular (see help pages for a complete description of argument of those functions)

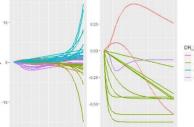
BMD plot

bmdplot(extendedres, add.CI, facetby, facetby2, shapeby, colorby, add.label, BMD log transfo)

BMD plot with gradient







Dose-response curves plot

curvesplot(extendedres, xmin, xmax, facetby, facetby2, colorby, dose_log_transfo = FALSE)

Trend plot

trendplot(extendedres, group, facetby)

Translation

Signal barackudion

Used metabolism

Lipid metabo

Sensitivity plot

Cartolystate metabolismCartolystate metabolismSensitivityplot (
Exactationextendedres, group,
colorby, BMDsummary =
C("first.quartile",
"median",
"median",
"median.and.IQR"),
BMD_log_transfo)

Americand metabolismLigid metabolism-