DRomics :: CHEAT SHEET

Written by the authors of the DRomics package - Updated in june 2024
See https://lbbe.univ-lyon1.fr/fr/dromics

Format of data

Data can be imported from a **.txt file** 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 as input, corresponding to the output of `read.table(file, header = FALSE)` on a file described as above.
`formatdata4DRomics()` can be used to help formatting such an R object.

Identifiers of items (contigs, probes, metabolites, ...)

RefSeq	0	0	0.22	0.2
NM_144958	2072	2506	2519	211
NR_102758	0	0	0	
NM_172405	198	265	250	24
NM_029777	18	29	25	1
NM_0011301	0	0	0	
NM_0011623	3	1	2	
NM_008117	0	0	0	
NM_0011682	61	65	79	8
NM_010910	7	10	9	
NR_002862	139	172	165	15
NR_033520	318	407	425	43

Tested doses or concentrations

Signal (counts of reads,continuous signal in log2, ...)

Workflow for analysis of data

See below the functions with their main arguments (see help pages for their complete description).

Step 1: import, check and pretreatment

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

PCAdataplot(omicdata, batch, label)
```

Step 2: selection of significantly responsive items

```
itemselect(omicdata, select.method = c("quadratic", "linear", "ANOVA"),
  FDR = 0.05)
```

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)
```

Step 5: bootstrap to compute BMD confidence intervals

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

Typical script for the workflow

```
o <- RNAseq(datafilename)
PCAdataplot(o)
s <- itemselect(o)
f <- drcfit(s)
r <- bmdcalc(f)
b <- bmdboot(r)
b$res
```

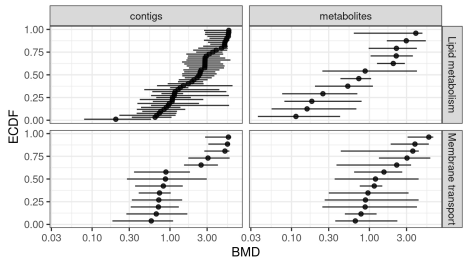
Each function of this workflow returns a S3 class object that can be printed and plotted using `print()` and `plot()` functions. Targetted items can be explored whatever they are or not in the selection using `targetplot(items, f)`.

Other functions to help the interpretation of results within a multi-level approach using a unique biological annotation

Functions taking as a first argument `extendedres`, a dataframe with the main workflow results, optionally gathering results obtained at different experimental (different molecular levels, different time points, different pre-exposure histories, ...) extended with additional columns coding for the biological annotation of items and optionally for the experimental level. Some lines of the workflow results can be replicated for items having more than one annotation. The `selectgroups()` and `bmdfilter()` functions can be used to focus on groups or items before producing the plot. See help pages for a complete description of functions illustrated below.

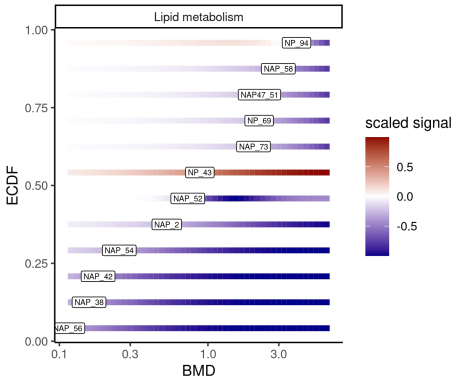
BMD plot

```
bmdplot(extendedres, add.CI, facetby,
  facetby2, shapeby, colorby,
  add.label, BMD_log_transfo)
```



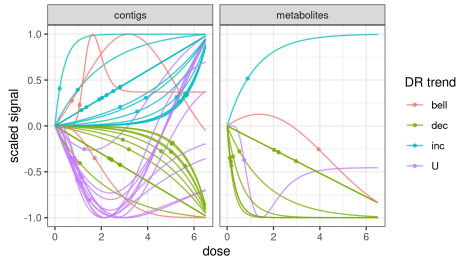
BMD plot with gradient

```
bmdplotwithgradient(extendedres, xmin,
  xmax, scaling, facetby, facetby2,
  shapeby, line.size, add.label,
  BMD_log_transfo)
```



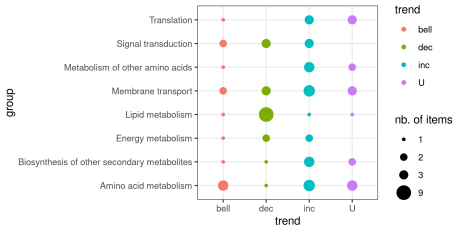
Dose-response curves plot

```
curvesplot(extendedres, xmin, xmax,
  scaling, facetby, facetby2, colorby,
  line.size, dose_log_transfo, addBMD)
```



Trend plot

```
trendplot(extendedres, group, facetby)
```



Sensitivity plot

```
sensitivityplot(extendedres, group,
  colorby, BMDsummary =
  c("first.quartile", "median",
  "median.and.IQR"), BMD_log_transfo)
```