

## Workflow metabolite set enrichment analysis with bootstrapping

```
options(stringsAsFactors = FALSE, warn = -1)

## install devtools if not installed
if(!("devtools" %in% rownames(installed.packages()))){
  install.packages("devtools", repos = c(CRAN = "http://cran.rstudio.com"))
}

## install bmetenrichr if not installed
if(!("bmetenrichr" %in% rownames(installed.packages()))){
  devtools::install_github(repo = "martijnmolenaar/bmetenrichr", build_vignettes = TRUE)
}

library(bmetenrichr)
#> Loading required package: ggplot2
#> Loading required package: dplyr
#>
#> Attaching package: 'dplyr'
#> The following objects are masked from 'package:stats':
#>
#>   filter, lag
#> The following objects are masked from 'package:base':
#>
#>   intersect, setdiff, setequal, union
```

load example data

```
data("Rappez_et_al")
```

create object

```
myTestRun <-
  initEnrichment(scmatrix = Rappez_et_al$sc_matrix,
                 annotations = rownames(Rappez_et_al$sc_matrix),
                 conditions = Rappez_et_al$conditions,
                 include = Rappez_et_al$cellular,
                 condition.x = "U",
                 condition.y = "F"
  )

#>
#> Parsing isomers...
#> single-cell metabolomics matrix of 3385 metabolites and 8807 cells
#> active pathway: LION
#>
#> conditions: F, FI, FIT, U
#>
#> condition.x: U
#> condition.y: F
```

```
## rank metabolites, in this case by t.test statistic

myTestRun <- rankScore(myTestRun, ranking.by = 't.test')
#> number of ties: 19 (1.73%)

## perform enrichment analysis with n = 100 bootstraps

myTestRun <- calcEnrichment(myTestRun, n = 100)
#>
#> Bootstrapping...
#>
#> Match to pathway...
#> 35.43% of annotations were matched to pathway
#>
#> Perform enrichment analysis...

## plot enrichment analysis, with enrichment score (ES) on x-axis

plotEnrichment(myTestRun, min.annotations = 5, q.value.cutoff = .05, by.statistic = "ES")
```

