

Package ‘autonomics’

December 11, 2023

Type Package

Title Generifying and intuifying cross-platform omics analysis

Version 1.10.2

Description

This package offers a generic and intuitive solution for cross-platform omics data analysis. It has functions for import, preprocessing, exploration, contrast analysis and visualization of omics data. It follows a tidy, functional programming paradigm.

License GPL-3

Encoding UTF-8

LazyData true

VignetteBuilder knitr

biocViews DataImport, DimensionReduction, GeneExpression, MassSpectrometry, Preprocessing, PrincipalComponent, RNASeq, Software, Transcription

BugReports <https://bitbucket.org/graumannlabtools/autonomics>

URL <https://github.com/bhagwataditya/autonomics>

RoxygenNote 7.2.4

Depends R (>= 4.0)

Imports abind, assertive.base, assertive.files, assertive.numbers, assertive.sets, BiocFileCache, BiocGenerics, bit64, colorspace, data.table, dplyr, edgeR, ggplot2, ggrepel, graphics, grDevices, grid, gridExtra, limma, magrittr, matrixStats, methods, MultiAssayExperiment, parallel, pcaMethods, rappdirs, rlang, R.utils, readxl, S4Vectors, scales, stats, stringi, SummarizedExperiment, tidy, tools, utils

Suggests affy, AnnotationDbi, BiocManager, BiocStyle, diagram, GenomicRanges, GEOquery, hgu95av2.db, ICSNP, knitr, lme4, lmerTest, MASS, mixOmics, mpm, nlme, org.Hs.eg.db, org.Mm.eg.db, RCurl, remotes, rmarkdown, ropls, Rsubread, rtracklayer, seqinr, statmod, testthat

git_url <https://git.bioconductor.org/packages/autonomics>

git_branch RELEASE_3_18

git_last_commit 230045c

git_last_commit_date 2023-11-08

Repository Bioconductor 3.18

Date/Publication 2023-12-11

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| | |
|----------------|--|
| .read_maxquant | <i>Read/Analyze proteingroups/phosphosites</i> |
|----------------|--|

Description

Read/Analyze proteingroups/phosphosites

Usage

```
.read_maxquant(
  file,
  quantity = guess_maxquant_quantity(file),
  sfile = NULL,
  sfileby = NULL,
  subgroupvar = "subgroup",
  select_subgroups = NULL,
  invert_subgroups = character(0),
  pepcountpattern = MAXQUANT_PATTERNS_PEPCOUNTS[1],
  verbose = TRUE
)
```

```
read_proteingroups(  
  file,  
  quantity = guess_maxquant_quantity(file),  
  sfile = NULL,  
  sfileby = NULL,  
  select_subgroups = NULL,  
  contaminants = FALSE,  
  reverse = FALSE,  
  fastafile = NULL,  
  invert_subgroups = character(0),  
  impute = stri_detect_regex(quantity, "[Ii]ntensity"),  
  pepcountpattern = MAXQUANT_PATTERNS_PEP_COUNTS[1],  
  subgroupvar = NULL,  
  formula = NULL,  
  block = NULL,  
  contrastdefs = NULL,  
  pca = FALSE,  
  fit = NULL,  
  verbose = TRUE,  
  plot = TRUE  
)  
  
read_phosphosites(  
  file,  
  proteinfile = paste0(dirname(file), "/proteinGroups.txt"),  
  quantity = guess_maxquant_quantity(file),  
  sfile = NULL,  
  sfileby = NULL,  
  select_subgroups = NULL,  
  contaminants = FALSE,  
  reverse = FALSE,  
  min_localization_prob = 0.75,  
  fastafile = NULL,  
  invert_subgroups = character(0),  
  pca = FALSE,  
  fit = NULL,  
  subgroupvar = NULL,  
  formula = NULL,  
  block = NULL,  
  contrastdefs = NULL,  
  verbose = TRUE,  
  plot = TRUE  
)
```

Arguments

file proteingroups/phosphosites file

| | |
|-----------------------|--|
| quantity | string: "Ratio normalized", "Ratio", "LFQ intensity", "Reporter intensity corrected", "Reporter intensity", "Intensity labeled", "Intensity" |
| sfile | sample file |
| sfileby | sample file mergeby column |
| subgroupvar | subgroup svar |
| select_subgroups | subgroups to be selected (character vector) |
| invert_subgroups | subgroups to be inverted (character vector) |
| pepcountpattern | value in MAXQUANT_PATTERNS_PEP COUNTS |
| verbose | whether to message |
| contaminants | whether to return contaminants |
| reverse | whether to return reverse peptides |
| fastafile | NULL or fastafile (to deconvolute proteingroups) |
| impute | whether to impute consistent nondetects |
| formula | desgnmat formula |
| block | block svar |
| contrastdefs | contrastdef vector/matrix/list |
| pca | whether to pca |
| fit | fit model: NULL, 'limma', 'lm', 'lme', 'lmer', 'wilcoxon' |
| plot | whether to plot |
| proteinfile | proteingroups file |
| min_localization_prob | min site localization probability (number) |

Value

SummarizedExperiment

Examples

```
file <- download_data('fukuda20.proteingroups.txt')
object <- read_proteingroups(file, pca=TRUE, fit='limma')
```

| | |
|-----------------|-----------------------|
| .read_metabolon | <i>Read metabolon</i> |
|-----------------|-----------------------|

Description

Read metabolon

Usage

```
.read_metabolon(  
  file,  
  sheet = "OrigScale",  
  fid_var = "(COMP|COMP_ID)",  
  sid_var = "(CLIENT_IDENTIFIER|Client ID)",  
  sfile = NULL,  
  sfileby = NULL,  
  by = NULL,  
  subgroupvar = "Group"  
)
```

```
read_metabolon(  
  file,  
  sheet = "OrigScale",  
  fid_var = "(COMP|COMP_ID)",  
  sid_var = "(CLIENT_IDENTIFIER|Client ID)",  
  sfile = NULL,  
  sfileby = NULL,  
  by = NULL,  
  subgroupvar = "Group",  
  fname_var = "BIOCHEMICAL",  
  impute = FALSE,  
  add_kegg_pathways = FALSE,  
  add_smiles = FALSE,  
  pca = FALSE,  
  fit = NULL,  
  formula = NULL,  
  block = NULL,  
  contrastdefs = NULL,  
  verbose = TRUE,  
  plot = TRUE  
)
```

Arguments

| | |
|-------|--------------------------|
| file | metabolon xlsx filepath |
| sheet | xls sheet number or name |

| | |
|-------------------|---|
| fid_var | feature_id fvar |
| sid_var | sampleid svar |
| sfile | sample file |
| sfileby | sample file mergeby column |
| by | metabolon file mergeby column |
| subgroupvar | subgroup svar |
| fname_var | featurename fvar |
| impute | whether to impute |
| add_kegg_pathways | whether to add kegg pathways |
| add_smiles | whether to add smiles |
| pca | whether to pca |
| fit | fit model: NULL, 'limma', 'lm', 'lme', 'lmer', 'wilcoxon' |
| formula | designmat formula |
| block | block svar |
| contrastdefs | contrastdef vector/matrix/list |
| verbose | whether to msg |
| plot | whether to plot |

Value

SummarizedExperiment

Examples

```
file <- download_data('atkin18.metabolon.xlsx')
read_metabolon(file, pca = TRUE, fit = 'limma', block='SUB')
```

.read_rectangles

Read omics data from rectangular file

Description

Read omics data from rectangular file

Usage

```
.read_rectangles(  
  file,  
  sheet = 1,  
  fid_rows,  
  fid_cols,  
  sid_rows,  
  sid_cols,  
  expr_rows,  
  expr_cols,  
  fvar_rows = NULL,  
  fvar_cols = NULL,  
  svar_rows = NULL,  
  svar_cols = NULL,  
  fdata_rows = NULL,  
  fdata_cols = NULL,  
  sdata_rows = NULL,  
  sdata_cols = NULL,  
  transpose = FALSE,  
  verbose = TRUE  
)  
  
read_rectangles(  
  file,  
  sheet = 1,  
  fid_rows,  
  fid_cols,  
  sid_rows,  
  sid_cols,  
  expr_rows,  
  expr_cols,  
  fvar_rows = NULL,  
  fvar_cols = NULL,  
  svar_rows = NULL,  
  svar_cols = NULL,  
  fdata_rows = NULL,  
  fdata_cols = NULL,  
  sdata_rows = NULL,  
  sdata_cols = NULL,  
  transpose = FALSE,  
  sfile = NULL,  
  sfileby = NULL,  
  subgroupvar = character(0),  
  verbose = TRUE  
)
```

Arguments

| | |
|--------------------------|--|
| <code>file</code> | string: name of text (txt, csv, tsv, adat) or excel (xls, xlsx) file |
| <code>sheet</code> | integer/string: only relevant for excel files |
| <code>fid_rows</code> | numeric vector: featureid rows |
| <code>fid_cols</code> | numeric vector: featureid cols |
| <code>sid_rows</code> | numeric vector: sampleid rows |
| <code>sid_cols</code> | numeric vector: sampleid cols |
| <code>expr_rows</code> | numeric vector: expr rows |
| <code>expr_cols</code> | numeric vector: expr cols |
| <code>fvar_rows</code> | numeric vector: fvar rows |
| <code>fvar_cols</code> | numeric vector: fvar cols |
| <code>svar_rows</code> | numeric vector: svar rows |
| <code>svar_cols</code> | numeric vector: svar cols |
| <code>fdata_rows</code> | numeric vector: fdata rows |
| <code>fdata_cols</code> | numeric vector: fdata cols |
| <code>sdata_rows</code> | numeric vector: sdata rows |
| <code>sdata_cols</code> | numeric vector: sdata cols |
| <code>transpose</code> | TRUE or FALSE (default) |
| <code>verbose</code> | TRUE (default) or FALSE |
| <code>sfile</code> | sample file |
| <code>sfileby</code> | sample file mergeby column |
| <code>subgroupvar</code> | subgroupvar in sfile |

Value

SummarizedExperiment

Examples

```
# RNASEQ
file <- download_data('billing16.rnacounts.txt')
read_rectangles(file, fid_rows = 2:58736, fid_cols = 1,
                sid_rows = 1, sid_cols = 4:14,
                expr_rows = 2:58736, expr_cols = 4:14,
                fvar_rows = 1, fvar_cols = 1:3,
                fdata_rows = 2:58736, fdata_cols = 1:3,
                transpose = FALSE)

# LCMSMS PROTEINGROUPS
file <- download_data('billing19.proteingroups.txt')
read_rectangles(file, fid_rows = 2:9044, fid_cols = 383,
                sid_rows = 1, sid_cols = seq(124, 316, by = 6),
                expr_rows = 2:9044, expr_cols = seq(124, 316, by = 6),
                fvar_rows = 1, fvar_cols = c(2, 6, 7, 383),
```

```
fdata_rows = 2:9044, fdata_cols = c(2, 6, 7, 383),
transpose = FALSE)
# SOMASCAN
file <- download_data('billing16.somascan.adat')
read_rectangles(file, fid_rows = 21, fid_cols = 19:1146,
  sid_rows = 30:40, sid_cols = 4,
  expr_rows = 30:40, expr_cols = 19:1146,
  fvar_rows = 21:28, fvar_cols = 18,
  svar_rows = 29, svar_cols = 1:17,
  fdata_rows = 21:28, fdata_cols = 19:1146,
  sdata_rows = 30:40, sdata_cols = 1:17,
  transpose = TRUE)
# METABOLON
file <- download_data('halama18.metabolon.xlsx')
read_rectangles(file, sheet = 2,
  fid_rows = 11:401, fid_cols = 5,
  sid_rows = 3, sid_cols = 15:86,
  expr_rows = 11:401, expr_cols = 15:86,
  fvar_rows = 10, fvar_cols = 1:14,
  svar_rows = 1:10, svar_cols = 14,
  fdata_rows = 11:401, fdata_cols = 1:14,
  sdata_rows = 1:10, sdata_cols = 15:86,
  transpose = FALSE)
```

.read_rnaseq_bams *Read rnaseq*

Description

Read/analyze rnaseq counts / bamfiles

Usage

```
.read_rnaseq_bams(
  dir,
  paired,
  genome,
  nthreads = detectCores(),
  sfile = NULL,
  sfileby = NULL,
  subgroupvar = NULL,
  ffile = NULL,
  ffileby = NULL,
  fnamevar = NULL,
  verbose = TRUE
)

.read_rnaseq_counts(
  file,
```

```
    fid_col = 1,
    sfile = NULL,
    sfileby = NULL,
    ffile = NULL,
    ffileby = NULL,
    subgroupvar = NULL,
    verbose = TRUE
)

read_rnaseq_bams(
  dir,
  paired,
  genome,
  nthreads = detectCores(),
  sfile = NULL,
  sfileby = NULL,
  subgroupvar = NULL,
  block = NULL,
  ffile = NULL,
  ffileby = NULL,
  fnamevar = NULL,
  formula = NULL,
  min_count = 10,
  pseudocount = 0.5,
  genesize = NULL,
  cpm = TRUE,
  tmm = cpm,
  log2 = TRUE,
  pca = FALSE,
  fit = NULL,
  voom = !is.null(fit),
  contrastdefs = NULL,
  verbose = TRUE,
  plot = TRUE
)

read_rnaseq_counts(
  file,
  fid_col = 1,
  sfile = NULL,
  sfileby = NULL,
  subgroupvar = NULL,
  block = NULL,
  ffile = NULL,
  ffileby = NULL,
  fnamevar = NULL,
  formula = NULL,
  min_count = 10,
```

```
pseudocount = 0.5,  
genesize = NULL,  
cpm = TRUE,  
tmm = cpm,  
log2 = TRUE,  
pca = FALSE,  
fit = NULL,  
voom = !is.null(fit),  
contrastdefs = NULL,  
verbose = TRUE,  
plot = TRUE  
)
```

Arguments

| | |
|--------------|--|
| dir | read_rnaseq_bams: bam/samfile dir |
| paired | read_rnaseq_bams: whether paired end reads |
| genome | read_rnaseq_bams: mm10/"hg38"/etc. or GTF file |
| nthreads | read_rnaseq_bams: nthreads used by Rsubread::featureCounts() |
| sfile | sample file |
| sfileby | sample file mergeby column |
| subgroupvar | subgroup svar |
| ffile | feature file |
| ffileby | feature file mergeby column |
| fnamevar | featurename fvar |
| verbose | whether to message |
| file | read_rnaseq_counts: count file |
| fid_col | featureid fvar |
| block | block svar |
| formula | designmat formula |
| min_count | min feature count required in some samples |
| pseudocount | added pseudocount to prevent -Inf log2 values |
| genesize | genesize fvar for tpm |
| cpm | whether to compute cpm |
| tmm | whether to tmm-scale library sizes |
| log2 | whether to log2 transform |
| pca | whether to pca |
| fit | fit model: NULL, 'limma', 'lm', 'lme', 'lmer', 'wilcoxon' |
| voom | whether to compute voom precision weights |
| contrastdefs | contrastdef vector/matrix/list |
| plot | whether to plot |

Value

SummarizedExperiment

Author(s)

Aditya Bhagwat, Shahina Hayat

Examples

```
file <- download_data('billing19.rnacounts.txt')
object <- read_rnaseq_counts(file, pca= TRUE, fit='limma')

# requires Rsubread
# file <- download_data('billing16.bam.zip')
# object <- read_rnaseq_bams(file, paired=TRUE, genome='hg38', pca=TRUE,
#                           fit='limma', plot=TRUE)
```

.read_somascan

Read somascan

Description

Read data from somascan adat file

Usage

```
.read_somascan(
  file,
  fidvar = "SeqId",
  sidvar = "SampleId",
  sfile = NULL,
  sfileby = NULL,
  by = NULL,
  subgroupvar = "SampleGroup"
)

read_somascan(
  file,
  fidvar = "SeqId",
  sidvar = "SampleId",
  sfile = NULL,
  sfileby = NULL,
  by = NULL,
  subgroupvar = "SampleGroup",
  fname_var = "EntrezGeneSymbol",
  sample_type = "Sample",
  feature_type = "Protein",
```

```
sample_quality = c("FLAG", "PASS"),  
feature_quality = c("FLAG", "PASS"),  
rm_na_svars = FALSE,  
rm_single_value_svars = FALSE,  
pca = FALSE,  
fit = NULL,  
formula = NULL,  
block = NULL,  
contrastdefs = NULL,  
verbose = TRUE,  
plot = TRUE  
)
```

Arguments

| | |
|-----------------------|--|
| file | *.adat file path (string) |
| fidvar | featureid fvar (string) |
| sidvar | sampleid svar (string) |
| sfile | sample file |
| sfileby | sample file mergeby column |
| by | metabolon file mergeby column |
| subgroupvar | subgroup svar (string) |
| fname_var | featurename fvar (string) |
| sample_type | subset of c('Sample', 'QC', 'Buffer', 'Calibrator') |
| feature_type | subset of c('Protein', 'Hybridization Control Elution', 'Rat Protein') |
| sample_quality | subset of c('PASS', 'FLAG', 'FAIL') |
| feature_quality | subset of c('PASS', 'FLAG', 'FAIL') |
| rm_na_svars | whether to rm NA svars |
| rm_single_value_svars | whether to rm single value svars |
| pca | whether to pca |
| fit | fit model: NULL, 'limma', 'lm', 'lme', 'lmer', 'wilcoxon' |
| formula | design formula (using svars) |
| block | block var |
| contrastdefs | contrastdef vector/matrix/list |
| verbose | whether to msg |
| plot | whether to plot |

Value

Summarizedexperiment

Examples

```
file <- download_data('atkin18.somascan.adat')
read_somascan(file, pca = TRUE, fit = 'limma', block = 'Subject_ID')
```

add_smiles*Add smiles*

Description

Add smiles

Usage

```
add_smiles(object)
```

Arguments

object character/factor vector with pubchem ids

Value

character/factor vector

References

<https://pubchemdocs.ncbi.nlm.nih.gov/pug-rest-tutorial>

Examples

```
file <- download_data('atkin18.metabolon.xlsx')
object <- read_metabolon(file, plot=FALSE)
add_smiles(object[1:10, ])
```

analysis*Get/set analysis*

Description

Get/set analysis

Usage

```

analysis(object)

## S4 method for signature 'SummarizedExperiment'
analysis(object)

analysis(object) <- value

## S4 replacement method for signature 'SummarizedExperiment,list'
analysis(object) <- value

```

Arguments

| | |
|--------|----------------------|
| object | SummarizedExperiment |
| value | list |

Value

analysis details (get) or updated object (set)

Examples

```

file <- download_data('billing16.proteingroups.txt')
object <- read_proteingroups(file, plot=FALSE)
analysis(object)

```

| | |
|---------|----------------|
| analyze | <i>Analyze</i> |
|---------|----------------|

Description

Analyze

Usage

```

analyze(
  object,
  pca = FALSE,
  fit = NULL,
  subgroupvar = default_subgroupvar(object),
  formula = default_formula(object, subgroupvar, fit),
  block = NULL,
  weightvar = if ("weights" %in% assayNames(object)) "weights" else NULL,
  contrastdefs = contrast_coefs(object, formula),
  verbose = TRUE,
  plot = TRUE
)

```

Arguments

| | |
|--------------|---|
| object | SummarizedExperiment |
| pca | whether to perform pca |
| fit | NULL, 'limma', 'lm', 'lme', 'lmer', or 'wilcoxon' |
| subgroupvar | subgroup svar |
| formula | model formula |
| block | block svar |
| weightvar | NULL or name of weight matrix in assays(object) |
| contrastdefs | contrastdefs vector/matrix/list |
| verbose | whether to msg |
| plot | whether to plot |

Value

SummarizedExperiment

Examples

```
require(magrittr)
file <- download_data('atkin18.metabolon.xlsx')
object <- read_metabolon(file, plot=FALSE)
object %<>% analyze(pca=TRUE, subgroupvar = 'Group', fit='limma')
```

assert_is_valid_sumexp

Assert that x is a valid SummarizedExperiment

Description

Assert that x is a valid SummarizedExperiment

Assert that x is a valid SummarizedExperiment

Usage

```
assert_is_valid_sumexp(x, .xname = get_name_in_parent(x))
```

```
assert_is_valid_sumexp(x, .xname = get_name_in_parent(x))
```

Arguments

| | |
|--------|--|
| x | SummarizedExperiment |
| .xname | see assertive.base::get_name_in_parent |

Value

TRUE or FALSE

TRUE or FALSE

Examples

```
# VALID
file <- download_data('halama18.metabolon.xlsx')
x <- read_metabolon(file, plot = FALSE)
assert_is_valid_sumexp(x)
# NOT VALID
rownames(SummarizedExperiment::colData(x)) <- NULL
# assert_is_valid_sumexp(x)
# VALID
file <- download_data('halama18.metabolon.xlsx')
x <- read_metabolon(file, plot = FALSE)
assert_is_valid_sumexp(x)
# NOT VALID
rownames(SummarizedExperiment::colData(x)) <- NULL
# assert_is_valid_sumexp(x)
```

AUTONOMICS_DATASETS *Data used in examples/vignette/tests/longtests*

Description

Data used in examples/vignette/tests/longtests

Usage

AUTONOMICS_DATASETS

Format

An object of class character of length 13.

Examples

AUTONOMICS_DATASETS

`biplot`*Biplot*

Description

Biplot

Usage

```
biplot(  
  object,  
  x = pca1,  
  y = pca2,  
  color = NULL,  
  group = NULL,  
  label = NULL,  
  feature_label = feature_name,  
  ...,  
  fixed = list(shape = 15, size = 3),  
  nloadings = 0  
)  
  
plot_biplot(...)
```

Arguments

| | |
|----------------------------|--|
| <code>object</code> | SummarizedExperiment |
| <code>x</code> | pca1, etc. |
| <code>y</code> | pca2, etc. |
| <code>color</code> | svar mapped to color (symbol) |
| <code>group</code> | svar mapped to group |
| <code>label</code> | svar mapped to label (symbol) |
| <code>feature_label</code> | fvar mapped to (loadings) label |
| <code>...</code> | additional svars mapped to aesthetics |
| <code>fixed</code> | fixed plot aesthetics |
| <code>nloadings</code> | number of loadings per half-axis to plot |

Value

ggplot object

Examples

```

require(magrittr)
file <- download_data('atkin18.metabolon.xlsx')
object <- read_metabolon(file, plot = FALSE)
object %<>% pca(ndim=4)
biplot(object)
biplot(object, color=SUB, group=SUB)
biplot(object, color=SUB, nloadings=1)
biplot(object, pca3, pca4, color=SUB, nloadings=1)

```

| | |
|--------|-----------------------|
| center | <i>Center samples</i> |
|--------|-----------------------|

Description

Center samples

Usage

```

center(
  object,
  selector = rep(TRUE, nrow(object)) == TRUE,
  fun = "median",
  verbose = TRUE
)

```

Arguments

| | |
|----------|--|
| object | SummarizedExperiment |
| selector | logical vector (length = nrow(object)) |
| fun | aggregation function (string) |
| verbose | TRUE/FALSE |

Value

SummarizedExperiment

Examples

```

require(magrittr)
require(matrixStats)
file <- download_data('fukuda20.proteingroups.txt')
object <- read_proteingroups(file, plot=FALSE, impute=FALSE)
fdata(object)$housekeeping <- FALSE
fdata(object)$housekeeping[order(rowVars(values(object)))[1:100]] <- TRUE
values(object)[, object$subgroup=='Adult'] %<>% add(5)
plot_sample_densities(object)
plot_sample_densities(center(object))
plot_sample_densities(center(object, housekeeping))

```

| | |
|--------------|-----------------------------|
| contrastdefs | <i>Get/set contrastdefs</i> |
|--------------|-----------------------------|

Description

Get/set contrastdefs

Usage

```
contrastdefs(object)

## S4 method for signature 'SummarizedExperiment'
contrastdefs(object)

contrastdefs(object) <- value

## S4 replacement method for signature 'SummarizedExperiment,list'
contrastdefs(object) <- value
```

Arguments

| | |
|--------|----------------------|
| object | SummarizedExperiment |
| value | list |

Value

contrastdefs (get) or SummarizedExperiment (set)

Examples

```
file <- download_data('billing16.proteingroups.txt')
inv <- c('EM_E', 'BM_E', 'BM_EM')
object <- read_proteingroups(
  file, invert_subgroups=inv, fit='limma', plot=FALSE)
contrastdefs(object)
```

| | |
|------------------------|--------------------------|
| contrast_subgroup_cols | <i>Row/Col contrasts</i> |
|------------------------|--------------------------|

Description

Row/Col contrasts

Usage

```
contrast_subgroup_cols(object, subgroupvar)
```

```
contrast_subgroup_rows(object, subgroupvar)
```

Arguments

object SummarizedExperiment

subgroupvar subgroup svar

Value

matrix

Examples

```
file <- download_data('halama18.metabolon.xlsx')
object <- read_metabolon(file, plot=FALSE)
subgroup_matrix(object, subgroupvar = 'Group')
contrast_subgroup_cols(object, subgroupvar = 'Group')
contrast_subgroup_rows(object, subgroupvar = 'Group')
```

counts

Get/Set counts

Description

Get / Set counts matrix

Usage

```
counts(object)
```

```
## S4 method for signature 'SummarizedExperiment'
counts(object)
```

```
counts(object) <- value
```

```
## S4 replacement method for signature 'SummarizedExperiment,matrix'
counts(object) <- value
```

```
## S4 replacement method for signature 'SummarizedExperiment,numeric'
counts(object) <- value
```

```
## S4 replacement method for signature 'SummarizedExperiment,`NULL`'
counts(object) <- value
```

Arguments

object SummarizedExperiment
 value count matrix (features x samples)

Value

count matrix (get) or updated object (set)

Examples

```
file <- download_data('billing19.rnacounts.txt')
object <- read_rnaseq_counts(file, plot=FALSE)
counts(object) <- values(object)
counts(object)[1:3, 1:3]
```

counts2cpm *Convert between counts and cpm*

Description

Convert between counts and cpm

Usage

```
counts2cpm(x, libsize = scaledlibsizes(x))

cpm2counts(x, libsize)
```

Arguments

x count/cpm matrix
 libsize (scaled) libsize vector

Value

cpm/tpm/count matrix

Examples

```
file <- download_data('billing19.rnacounts.txt')
object <- read_rnaseq_counts(file, cpm=FALSE, log2=FALSE, plot=FALSE)
libsize <- scaledlibsizes(values(object))
tpm <- counts2tpm(counts(object), genesize = 1)
cpm <- counts2cpm(counts(object), libsize)
counts <- cpm2counts(cpm, libsize)
sum(counts(object) - counts)
```

| | |
|------------|----------------------|
| counts2tpm | <i>counts to tpm</i> |
|------------|----------------------|

Description

counts to tpm

Usage

```
counts2tpm(x, genesize)
```

Arguments

| | |
|----------|----------------------------|
| x | count matrix |
| genesize | genesize vector (kilobase) |

Value

tpm matrix

Examples

```
file <- download_data('billing19.rnacounts.txt')
object <- read_rnaseq_counts(file, cpm=FALSE, log2=FALSE, plot=FALSE)
counts2tpm(counts(object), genesize=1)[1:3, 1:3]
```

| | |
|-----|--------------------|
| cpm | <i>Get/Set cpm</i> |
|-----|--------------------|

Description

Get / Set cpm matrix

Usage

```
cpm(object)

## S4 method for signature 'SummarizedExperiment'
cpm(object)

cpm(object) <- value

## S4 replacement method for signature 'SummarizedExperiment,matrix'
cpm(object) <- value

## S4 replacement method for signature 'SummarizedExperiment,numeric'
cpm(object) <- value
```

Arguments

| | |
|--------|---------------------------------|
| object | SummarizedExperiment |
| value | cpm matrix (features x samples) |

Value

cpm matrix (get) or updated object (set)

Examples

```
file <- download_data('billing19.rnacounts.txt')
object <- read_rnaseq_counts(file, plot=FALSE)
cpm(object) <- values(object)
cpm(object)[1:3, 1:3]
```

create_design

Create design

Description

Create design matrix for statistical analysis

Usage

```
create_design(
  object,
  subgroupvar = if ("subgroup" %in% svars(object)) "subgroup" else NULL,
  formula = default_formula(object, subgroupvar, fit = "limma"),
  verbose = TRUE
)
```

Arguments

| | |
|-------------|----------------------|
| object | SummarizedExperiment |
| subgroupvar | subgroup svar |
| formula | formula with svars |
| verbose | whether to message |

Value

design matrix

Examples

```

file <- download_data('billing19.rnacounts.txt')
object <- read_rnaseq_counts(file, plot=FALSE)
unique(create_design(object))

object$subgroup <- 'billing19'
unique(create_design(object))

file <- download_data('atkin18.somascan.adat')
object <- read_somascan(file, plot=FALSE)
unique(create_design(object))
create_design(object, formula= ~ 0 + SampleGroup + Sex + T2D + age + bmi)
object$subgroup <- 'atkin18'
unique(create_design(object))

```

| | |
|--------------|---------------------|
| create_sfile | <i>Create sfile</i> |
|--------------|---------------------|

Description

Create sfile

Usage

```
create_sfile(object, sfile, verbose = TRUE)
```

Arguments

| | |
|---------|----------------------|
| object | SummarizedExperiment |
| sfile | sample file |
| verbose | TRUE/FALSE |

Value

sample file path

Examples

```

file <- download_data('fukuda20.proteingroups.txt')
object <- read_proteingroups(file, plot=FALSE)
create_sfile(object, paste0(tempfile(), '.tsv'))

```

| | |
|---------------|----------------------|
| default_sfile | <i>Default sfile</i> |
|---------------|----------------------|

Description

Default sfile

Usage

```
default_sfile(file)
```

Arguments

| | |
|------|-----------|
| file | data file |
|------|-----------|

Value

sample file

Examples

```
file <- download_data('billing19.proteingroups.txt')
default_sfile(file)
```

| | |
|---------------------|-------------------------------|
| default_subgroupvar | <i>Create default formula</i> |
|---------------------|-------------------------------|

Description

Create default formula

Usage

```
default_subgroupvar(object)
```

```
default_formula(object, subgroupvar = default_subgroupvar(object), fit)
```

Arguments

| | |
|-------------|------------------------------|
| object | SummarizedExperiment |
| subgroupvar | string |
| fit | 'limma', 'lm', 'lme', 'lmer' |

Value

formula

Examples

```
file <- download_data('atkin18.metabolon.xlsx')
object <- .read_metabolon(file)
default_subgroupvar(object)
default_formula(object, fit = 'limma')
default_formula(object, fit = 'lm')
```

| | |
|---------------|---|
| download_data | <i>Download autonomics example data</i> |
|---------------|---|

Description

Download autonomics example data

Usage

```
download_data(
  filename,
  url = paste0("https://bitbucket.org/graumannlabtools/autonomics/downloads/", filename),
  verbose = TRUE
)
```

Arguments

| | |
|----------|---|
| filename | file name |
| url | web url |
| | <ul style="list-style-type: none"> • Billing 2016: stemcell comparison: E, EM, BM <ul style="list-style-type: none"> – 'billing16.bam.zip' – 'billing16.rnacounts.txt' – 'billing16.somascan.adat' – 'billing16.proteingroups.txt' • Atkin 2018: hypoglycemia: t0, t1, t2, t3 <ul style="list-style-type: none"> – 'atkin18.somascan.adat' – 'atkin18.metbolon.xlsx' • Halama 2018: glutaminase inhibition: 4 conc, 4 timepoints <ul style="list-style-type: none"> – 'halama18.metabolon.xlsx' • Billing 2019: stemcell differentiation: E00, E01, E02, E05, EM15, EM30, M00 <ul style="list-style-type: none"> – 'billing19.rnacounts.txt' – 'billing19.proteingroups.txt' – 'billing19.phosphosites.txt' • Fukuda 2020: zebrafish development: X30dpt, Adult <ul style="list-style-type: none"> – 'fukuda20.proteingroups.txt' |
| verbose | TRUE / FALSE |

Value

local file path

Examples

```
# atkin18 - hypoglycemia - pubmed 30525282
  download_data('atkin18.somascan.adat')      # somascan intensities
  download_data('atkin18.metabolon.xlsx')     # metabolon intensities

# billing16 - stemcell characterization - pubmed 26857143
  download_data('billing16.proteingroups.txt') # proteingroup ratios
  download_data('billing16.somascan.adat')     # somascan intensities
  download_data('billing16.rnacounts.txt')     # rnaseq counts
  download_data('billing16.bam.zip')          # rnaseq alignments

# billing19 - stemcell differentiation - pubmed 31332097
  # download_data('billing19.proteingroups.txt') # proteingroup ratios
  # download_data('billing19.phosphosites.txt')  # phosphosite ratios
  # download_data('billing19.rnacounts.txt')     # rnaseq counts

# fukuda20 - heart regeneration - pubmed PDX016235
  download_data('fukuda20.proteingroups.txt') # proteingroup LFQ

# halama18 - glutaminase inhibition - pubmed 30525282
  download_data('halama18.metabolon.xlsx')     # metabolon intensities
```

download_gtf

Download GTF file

Description

Download GTF file with feature annotations

Usage

```
download_gtf(
  organism,
  release = 100,
  gtffile = sprintf("%s/gtf/%s", rappdirs::user_cache_dir(appname = "autonomics"),
    basename(make_gtf_url(organism, release) %>% substr(1, nchar(.) - 3)))
)
```

Arguments

| | |
|----------|---|
| organism | 'Homo sapiens', 'Mus musculus' or 'Rattus norvegicus' |
| release | GTF release (number) |
| gtffile | string: path to local GTF file |

Value

gtffile path

Examples

```
organism <- 'Homo sapiens'  
# download_gtf(organism)
```

| | |
|--------|---------------------------------|
| dt2mat | <i>'data.table' to 'matrix'</i> |
|--------|---------------------------------|

Description

Convert between *'data.table'* and *'matrix'*

Usage

```
dt2mat(x)  
  
mat2dt(x, idvar)
```

Arguments

| | |
|-------|---------------------|
| x | data.table / matrix |
| idvar | idvar string |

Value

matrix / data.table

Examples

```
x <- data.table::data.table(  
  gene = c('ENSG001', 'ENSG002', 'ENSG003'),  
  sampleA = c(1787, 10, 432),  
  sampleB = c(1143, 3, 268))  
dt2mat(x)  
mat2dt(dt2mat(x), 'gene')
```

explore_imputations *Explore imputations*

Description

Explore imputations

Usage

```
explore_imputations(object, subgroup, xbiplot = pca1, ybiplot = pca2, ...)
```

Arguments

| | |
|----------|--------------------------------------|
| object | SummarizedExperiment |
| subgroup | subgroup (sym) |
| xbiplot | biplot x axis. Default pca1 (symbol) |
| ybiplot | biplot y axis. Default pca2 (symbol) |
| ... | aesthetic mappings |

Value

ggplot object

Examples

```
file <- download_data('fukuda20.proteingroups.txt')
object <- read_proteingroups(file, impute = FALSE, pca = TRUE, plot = FALSE)
explore_imputations(object, subgroup=subgroup)
explore_transformations(object, subgroup=subgroup)
```

explore_transformations *Explore transformations*

Description

Explore transformations

Usage

```

explore_transformations(
  object,
  subgroup = subgroup,
  transformations = c("quantnorm", "zscore", "invnorm"),
  method = "pca",
  xdim = 1,
  ydim = 2,
  ...
)

```

Arguments

| | |
|-----------------|-------------------------------|
| object | SummarizedExperiment |
| subgroup | subgroup (sym) |
| transformations | vector |
| method | 'pca', 'pls', 'sma', or 'lda' |
| xdim | number (default 1) |
| ydim | number (default 2) |
| ... | passed to plot_data |

Value

grid object

Examples

```

file <- download_data('billing16.proteingroups.txt')
invert <- c('EM_E', 'EM_BM', 'BM_E')
object <- read_proteingroups(file, invert_subgroups = invert, plot=FALSE)
explore_transformations(object)

```

| | |
|------------------|-------------------------|
| extract_features | <i>Extract features</i> |
|------------------|-------------------------|

Description

Extract features

Usage

```
extract_features(object, extractor)
```

Arguments

object SummarizedExperiment
extractor logical/numeric vector

Value

SummarizedExperiment

Examples

```
require(magrittr)
file <- download_data('billing16.proteingroups.txt')
object <- read_proteingroups(file, plot=FALSE)
(object %<>% extract_features(c(5,4)))
```

extract_rectangle *Extract rectangle from omics file, data.table, or matrix*

Description

Extract rectangle from omics file, data.table, or matrix

Usage

```
extract_rectangle(x, ...)
```

```
## S3 method for class 'character'
extract_rectangle(
  x,
  rows = seq_len(nrows(x, sheet = sheet)),
  cols = seq_len(ncols(x, sheet = sheet)),
  verbose = FALSE,
  transpose = FALSE,
  drop = FALSE,
  sheet = 1,
  ...
)
```

```
## S3 method for class 'data.table'
extract_rectangle(
  x,
  rows = seq_len(nrow(x)),
  cols = seq_len(ncol(x)),
  transpose = FALSE,
  drop = FALSE,
  ...
)
```

```
## S3 method for class 'matrix'
extract_rectangle(
  x,
  rows = seq_len(nrow(x)),
  cols = seq_len(ncol(x)),
  transpose = FALSE,
  drop = FALSE,
  ...
)
```

Arguments

| | |
|-----------|------------------------------|
| x | omics datafile or datatable |
| ... | allow for S3 method dispatch |
| rows | numeric vector |
| cols | numeric vector |
| verbose | logical |
| transpose | logical |
| drop | logical |
| sheet | numeric or string |

Value

matrix

Examples

```
# FROM FILE: extract_rectangle.character
#=====
# exprs
require(magrittr)
x <- download_data('halama18.metabolon.xlsx')
extract_rectangle(x, rows = 11:401, cols = 15:86, sheet = 2) %>%
  extract(1:3, 1:3)

# fids
extract_rectangle(x, rows = 11:401, cols = 5, sheet = 2) %>%
  extract(1:3, )

# sids
extract_rectangle(x, rows = 2, cols = 15:86, sheet = 2) %>%
  extract(,1:3)

# fdata
extract_rectangle(x, rows = 10:401, cols = 1:14, sheet = 2) %>%
  extract(1:3, 1:3)

# sdata
```

```

extract_rectangle(x, rows = 1:10, cols = 14:86, sheet = 2,
transpose = TRUE) %>% extract(1:3, 1:3)

# FROM MATRIX: extract_rectangle.matrix
#=====
# exprs
x <-download_data('halama18.metabolon.xlsx') %>%
  extract_rectangle(sheet = 2)
extract_rectangle(x, rows = 11:401, cols = 15:86, sheet = 2) %>%
  extract(1:3, 1:3)

# fids
extract_rectangle(x, rows = 11:401, cols = 5, sheet = 2) %>%
  extract(1:3, )

# sids
extract_rectangle(x, rows = 2, cols = 15:86, sheet = 2) %>%
  extract(,1:3)

# fdata
extract_rectangle(x, rows = 10:401, cols = 1:14, sheet = 2) %>%
  extract(1:3, 1:3)

# sdata
extract_rectangle(x, rows = 1:10, cols = 14:86, sheet = 2,
transpose = TRUE) %>% extract(1:3, 1:3)

```

fdata

Get/Set fdata

Description

Get/Set feature data

Usage

```
fdata(object)
```

```
## S4 method for signature 'SummarizedExperiment'
fdata(object)
```

```
fdata(object) <- value
```

```
## S4 replacement method for signature 'SummarizedExperiment,data.frame'
fdata(object) <- value
```

Arguments

| | |
|--------|--------------------------------------|
| object | SummarizedExperiment, eSet, or EList |
| value | data.frame |

Value

feature dataframe (get) or updated object (set)

Examples

```
require(magrittr)
file <- download_data('billing16.proteingroups.txt')
object <- read_proteingroups(file, plot=FALSE)
head(fdata(object)) # Getter
fdata(object) %<>% cbind(z=1)
head(fdata(object)) # Setter
```

filter_exprs_replicated_in_some_subgroup

Filter features with replicated expression in some subgroup

Description

Filter features with replicated expression in some subgroup

Usage

```
filter_exprs_replicated_in_some_subgroup(
  object,
  subgroupvar = "subgroup",
  comparator = if (contains_ratios(object)) "!=" else ">",
  lod = 0,
  verbose = TRUE
)
```

Arguments

| | |
|-------------|----------------------------|
| object | SummarizedExperiment |
| subgroupvar | subgroup svar |
| comparator | '>' or '!=' |
| lod | number: limit of detection |
| verbose | TRUE or FALSE |

Value

Filtered SummarizedExperiment

Examples

```
require(magrittr)
file <- download_data('atkin18.metabolon.xlsx')
object <- read_metabolon(file, plot=FALSE)
object %<>% filter_exprs_replicated_in_some_subgroup(subgroupvar = 'Group')
filter_exprs_replicated_in_some_subgroup(object, character(0))
filter_exprs_replicated_in_some_subgroup(object, NULL)
```

| | |
|-----------------|-------------------------------------|
| filter_features | <i>Filter features on condition</i> |
|-----------------|-------------------------------------|

Description

Filter features on condition

Usage

```
filter_features(object, condition, verbose = FALSE)
```

Arguments

| | |
|-----------|----------------------|
| object | SummarizedExperiment |
| condition | filter condition |
| verbose | logical |

Value

filtered eSet

Examples

```
file <- download_data('atkin18.metabolon.xlsx')
object <- read_metabolon(file, plot=FALSE)
filter_features(object, SUPER_PATHWAY=='Lipid', verbose = TRUE)
```

| | |
|---------------|-----------------------------|
| filter_medoid | <i>Filter medoid sample</i> |
|---------------|-----------------------------|

Description

Filter medoid sample

Usage

```
filter_medoid(object, by = NULL, verbose = FALSE)
```

Arguments

| | |
|---------|----------------------|
| object | SummarizedExperiment |
| by | svar |
| verbose | whether to message |

Value

SummarizedExperiment

Examples

```
require(magrittr)
file <- download_data('billing19.rnacounts.txt')
object <- read_rnaseq_counts(file, plot=FALSE)
object %<>% filter_medoid(by = 'subgroup', verbose=TRUE)
```

| | |
|-------------------|---------------------------------------|
| filter_replicated | <i>Filter for replicated features</i> |
|-------------------|---------------------------------------|

Description

Filter for replicated features

Usage

```
filter_replicated(object, comparator = `>`, lod = 0, n = 2, verbose = TRUE)
```

Arguments

| | |
|------------|--|
| object | SummarizedExperiment |
| comparator | string |
| lod | number: limit of detection |
| n | number: number of replicates above lod |
| verbose | TRUE/FALSE |

Value

SummarizedExperiment

Examples

```
require(magrittr)
file <- download_data('fukuda20.proteingroups.txt')
object <- read_proteingroups(file, plot=FALSE)
object %<>% filter_replicated()
```

| | |
|----------------|------------------------------------|
| filter_samples | <i>Filter samples on condition</i> |
|----------------|------------------------------------|

Description

Filter samples on condition

Usage

```
filter_samples(object, condition, verbose = FALSE, record = TRUE)
```

Arguments

| | |
|-----------|-------------------------|
| object | SummarizedExperiment |
| condition | filter condition |
| verbose | TRUE or FALSE (default) |
| record | TRUE (default) or FALSE |

Value

filtered SummarizedExperiment

Examples

```
file <- download_data('atkin18.metabolon.xlsx')
object <- read_metabolon(file, plot=FALSE)
filter_samples(object, Group != 't0', verbose = TRUE)
```

`fit_limma`*Fit model and test for differential expression*

Description

Fit model and test for differential expression

Usage

```
fit_limma(  
  object,  
  subgroupvar = if ("subgroup" %in% svars(object)) "subgroup" else NULL,  
  formula = default_formula(object, subgroupvar, "limma"),  
  contrastdefs = contrast_coefs(object, formula),  
  block = NULL,  
  weightvar = if ("weights" %in% assayNames(object)) "weights" else NULL,  
  verbose = TRUE,  
  plot = FALSE  
)
```

```
fit_lm(  
  object,  
  subgroupvar = if ("subgroup" %in% svars(object)) "subgroup" else NULL,  
  formula = default_formula(object, subgroupvar, fit = "lm"),  
  block = NULL,  
  weightvar = if ("weights" %in% assayNames(object)) "weights" else NULL,  
  contrastdefs = NULL,  
  verbose = TRUE,  
  plot = FALSE  
)
```

```
fit_lme(  
  object,  
  subgroupvar = if ("subgroup" %in% svars(object)) "subgroup" else NULL,  
  formula = default_formula(object, subgroupvar, fit = "lme"),  
  block = NULL,  
  weightvar = if ("weights" %in% assayNames(object)) "weights" else NULL,  
  contrastdefs = NULL,  
  verbose = TRUE,  
  plot = FALSE  
)
```

```
fit_lmer(  
  object,  
  subgroupvar = if ("subgroup" %in% svars(object)) "subgroup" else NULL,  
  formula = default_formula(object, subgroupvar, fit = "lmer"),  
  block = NULL,
```

```

weightvar = if ("weights" %in% assayNames(object)) "weights" else NULL,
contrastdefs = NULL,
verbose = TRUE,
plot = FALSE
)

fit_wilcoxon(
  object,
  subgroupvar = if ("subgroup" %in% svars(object)) "subgroup" else NULL,
  formula = default_formula(object, subgroupvar, fit = "wilcoxon"),
  contrastdefs = contrast_coefs(object, formula = formula),
  block = NULL,
  weightvar = NULL,
  verbose = TRUE,
  plot = FALSE
)

```

Arguments

| | |
|--------------|---|
| object | SummarizedExperiment |
| subgroupvar | subgroup variable |
| formula | modeling formula |
| contrastdefs | contrastdef vector / matrix / list <ul style="list-style-type: none"> • <code>c("t1-t0", "t2-t1", "t3-t2")</code> • <code>matrix(c("WT.t1-WT.t0", "WT.t2-WT.t1", "WT.t3-WT.t2"), c("KD.t1-KD.t0", "KD.t2-KD.t1", "KD.t3-KD.t2"), nrow=2, byrow=TRUE)</code> • <code>list(matrix(c("WT.t1-WT.t0", "WT.t2-WT.t1", "WT.t3-WT.t2"), c("KD.t1-KD.t0", "KD.t2-KD.t1", "KD.t3-KD.t2"), nrow=2, byrow=TRUE), matrix(c("KD.t0-WT.t0", "KD.t1-WT.t1", "KD.t2-WT.t2", "KD.t3-WT.t3"), nrow=1, byrow=TRUE))</code> |
| block | block svar (or NULL) |
| weightvar | NULL or name of weight matrix in <code>assays(object)</code> |
| verbose | whether to msg |
| plot | whether to plot |

Value

Updated SummarizedExperiment

Examples

```

require(magrittr)
file <- download_data('atkin18.somascan.adat')
object <- read_somascan(file, plot=FALSE)
object %<>% fit_limma(subgroupvar = 'SampleGroup')
object %<>% fit_lm( subgroupvar = 'SampleGroup')
plot_venn(is_sig(object, contrast='t3-t2'))

```

```

S4Vectors::metadata(object)$limma <- S4Vectors::metadata(object)$lm <- NULL
object %<>% fit_limma( subgroupvar = 'SampleGroup', block = 'Subject_ID')
object %<>% fit_wilcoxon(subgroupvar = 'SampleGroup', block = 'Subject_ID')
# object %<>% fit_lme( subgroupvar = 'SampleGroup', block = 'Subject_ID')
# object %<>% fit_lmer( subgroupvar = 'SampleGroup', block = 'Subject_ID')
plot_venn(is_sig(object, contrast='t3-t2'))

```

flevels

Get fvar levels

Description

Get fvar levels

Usage

```
flevels(object, fvar)
```

Arguments

| | |
|--------|----------------------|
| object | SummarizedExperiment |
| fvar | feature variable |

Value

fvar values

Examples

```

file <- download_data('billing16.proteingroups.txt')
object <- read_proteingroups(file, plot=FALSE)
head(flevels(object, 'feature_name'))

```

fnames

Get/Set fnames

Description

Get/Set feature names

Usage

```
fnames(object)

## S4 method for signature 'SummarizedExperiment'
fnames(object)

fnames(object) <- value

## S4 replacement method for signature 'SummarizedExperiment,character'
fnames(object) <- value
```

Arguments

| | |
|--------|--------------------------------------|
| object | SummarizedExperiment, eSet, or EList |
| value | character vector with feature names |

Value

feature name vector (get) or updated object (set)

Examples

```
require(magrittr)
file <- download_data('billing16.proteingroups.txt')
object <- read_proteingroups(file, plot=FALSE)
fnames(object) %<>% paste0('PG', .)
object
```

formula2str

formula to string

Description

formula to string

Usage

```
formula2str(formula)
```

Arguments

| | |
|---------|---------|
| formula | formula |
|---------|---------|

Value

string

Examples

```
formula2str(~0+subgroup)
```

fvalues

Get fvalues

Description

Get fvar values

Usage

```
fvalues(object, fvar)
```

Arguments

| | |
|--------|----------------------|
| object | SummarizedExperiment |
| fvar | feature variable |

Value

fvar values

Examples

```
file <- download_data('billing16.proteingroups.txt')
object <- read_proteingroups(file, plot=FALSE)
head(fvalues(object, 'feature_name'))
fvalues(object, NULL)
```

fvars

Get/Set fvars

Description

Get/Set feature variables

Usage

```
fvars(object)
```

```
## S4 method for signature 'SummarizedExperiment'
fvars(object)
```

```
fvars(object) <- value
```

```
## S4 replacement method for signature 'SummarizedExperiment,character'
fvars(object) <- value
```

Arguments

| | |
|--------|---|
| object | SummarizedExperiment |
| value | character vector with feature variables |

Value

feature variables vector (get) or updated object (set)

Examples

```
require(magrittr)
file <- download_data('billing16.proteingroups.txt')
object <- read_proteingroups(file, plot=FALSE)
fvars(object)[1] %<>% paste0('1')
fvars(object)[1]
```

guess_maxquant_quantity

Guess maxquant quantity from snames

Description

character vector, dataframe, or SummarizedExperiment.

Usage

```
guess_maxquant_quantity(x, ...)
```

```
## S3 method for class 'character'
guess_maxquant_quantity(x, ...)
```

```
## S3 method for class 'data.frame'
guess_maxquant_quantity(x, ...)
```

```
## S3 method for class 'SummarizedExperiment'
guess_maxquant_quantity(x, ...)
```

Arguments

| | |
|-----|--|
| x | character vector, dataframe, or SummarizedExperiment |
| ... | used for proper S3 method dispatch |

Value

string: value from names(MAXQUANT_PATTERNS_QUANTITY)

Examples

```
# file
file <- download_data('fukuda20.proteingroups.txt')
guess_maxquant_quantity(file)

# character vector
x <- "Ratio M/L normalized STD(L)_E00(M)_E01(H)_R1"
guess_maxquant_quantity(x)

x <- "Ratio M/L STD(L)_E00(M)_E01(H)_R1"
guess_maxquant_quantity(x)

x <- "LFQ intensity E00.R1"
guess_maxquant_quantity(x)

x <- "Reporter intensity corrected 0 STD(0)E00(1)E01(2)_R1"
guess_maxquant_quantity(x)

x <- "Reporter intensity 0 STD(0)E00(1)E01(2)_R1"
guess_maxquant_quantity(x)

x <- "Intensity H STD(L)_E00(M)_E01(H)_R1"
guess_maxquant_quantity(x)

# dataframe
file <- download_data('fukuda20.proteingroups.txt')
x <- data.table::fread(file)
guess_maxquant_quantity(x)

# SummarizedExperiment
file <- download_data('fukuda20.proteingroups.txt')
object <- read_proteingroups(file, plot=FALSE)
guess_maxquant_quantity(file)
```

guess_sep

Guess separator

Description

Guess separator

Usage

```
guess_sep(x, ...)
```

```
## S3 method for class 'character'
guess_sep(x, separators = c(".", "_"), verbose = FALSE, ...)
```

```
## S3 method for class 'factor'
```

```
guess_sep(x, ...)

## S3 method for class 'SummarizedExperiment'
guess_sep(x, var = "sample_id", separators = c(".", "_"), verbose = FALSE, ...)
```

Arguments

| | |
|------------|---|
| x | character vector or SummarizedExperiment |
| ... | used for proper S3 method dispatch |
| separators | character vector: possible separators to look for |
| verbose | TRUE or FALSE |
| var | svar or fvar |

Value

separator (string) or NULL (if no separator could be identified)

Examples

```
# charactervector
x <- c('PERM_NON.R1[H/L]', 'PERM_NON.R2[H/L]', 'PERM_NON.R3[H/L]')
guess_sep(x)

x <- c('WT untreated 1', 'WT untreated 2', 'WT treated 1')
guess_sep(x)

x <- c('group1', 'group2', 'group3.R1')
guess_sep(x)

# SummarizedExperiment
# file <- download_data('halama18.metabolon.xlsx')
# object <- read_metabolon(file, plot=FALSE)
# guess_sep(object)

# file <- download_data('billing16.proteingroups.txt')
# object <- read_proteingroups(file, plot=FALSE)
# guess_sep(object)
```

impute_systematic_nondetects

Impute systematic nondetects

Description

Impute systematic nondetects

Usage

```

impute_systematic_nondetects(
  object,
  subgroup = subgroup,
  fun = halfnormimpute,
  plot = TRUE,
  verbose = TRUE,
  ...
)

```

Arguments

| | |
|----------|----------------------|
| object | SummarizedExperiment |
| subgroup | subgroup svar |
| fun | imputation function |
| plot | TRUE or FALSE |
| verbose | TRUE or FALSE |
| ... | passed to 'fun' |

Value

SummarizedExperiment

Examples

```

file <- download_data('fukuda20.proteingroups.txt')
object <- read_proteingroups(file, impute = FALSE, plot = FALSE)
impute_systematic_nondetects(object)

```

| | |
|--------|---------------|
| invert | <i>Invert</i> |
|--------|---------------|

Description

For character vectors: invert collapsed strings. For SummarizedExperiments: invert expressions , subgroups, and sample ids

Usage

```

invert(x, ...)

## S3 method for class 'character'
invert(x, sep = guess_sep(x), ...)

## S3 method for class 'SummarizedExperiment'
invert(

```

```

x,
subgroups = slevels(x, "subgroup"),
sep = guess_sep(x, "subgroup"),
...
)

```

Arguments

```

x           character vector or SummarizedExperiment
...        to enable S3 method dispatch
sep        string: collapsed string separator
subgroups  character vector: subgroup levels to be inversed

```

Value

character vector or SummarizedExperiment

Examples

```

# character
x <- c('Ctrl_A', 'Ctrl_B')
invert(x)

# SummarizedExperiment
file <- download_data('fukuda20.proteingroups.txt')
object <- read_proteingroups(file, plot=FALSE)
invert(object)

```

| | |
|------------|---------------------------|
| is_imputed | <i>Get/set is_imputed</i> |
|------------|---------------------------|

Description

Get/Set is_imputed

Usage

```

is_imputed(object)

## S4 method for signature 'SummarizedExperiment'
is_imputed(object)

is_imputed(object) <- value

## S4 replacement method for signature 'SummarizedExperiment,matrix'
is_imputed(object) <- value

## S4 replacement method for signature 'SummarizedExperiment,`NULL`'
is_imputed(object) <- value

```

Arguments

| | |
|--------|----------------------|
| object | SummarizedExperiment |
| value | matrix |

Value

matrix (get) or updated object (set)

Examples

```
file <- download_data('billing16.proteingroups.txt')
object <- read_proteingroups(file, plot=FALSE)
sum(is_imputed(object))
```

| | |
|--------|------------------------|
| is_sig | <i>Is significant?</i> |
|--------|------------------------|

Description

Is significant?

Usage

```
is_sig(
  object,
  fit = intersect(names(metadata(object)), TESTS),
  contrast = if (is_scalar(fit)) colnames(metadata(object)[[fit]]) else 1,
  quantity = "fdr"
)
```

Arguments

| | |
|----------|---|
| object | SummarizedExperiment |
| fit | subset of autonomies::TESTS |
| contrast | subset of colnames(metadata(object)[[fit]]) |
| quantity | value in dimnames(metadata(object)[[fit]])[3] |

Value

matrix: -1 (downregulated), +1 (upregulatd), 0 (not fdr significant)

Examples

```
require(magrittr)
file <- download_data('fukuda20.proteingroups.txt')
object <- read_proteingroups(file, plot=FALSE)
object %<>% fit_lm()
object %<>% fit_limma()
issig <- is_sig(object, fit = c('lm','limma'), contrast = 'Adult-X30dpt')
plot_venn(issig)
```

limma

Get/set limma results

Description

Get/Set limma results

Usage

```
limma(object)

## S4 method for signature 'SummarizedExperiment'
limma(object)

limma(object) <- value

## S4 replacement method for signature 'SummarizedExperiment,array'
limma(object) <- value

## S4 replacement method for signature 'SummarizedExperiment,`NULL`'
limma(object) <- value
```

Arguments

| | |
|--------|----------------------|
| object | SummarizedExperiment |
| value | list |

Value

limma results (get) or updated object (set)

Examples

```
file <- download_data('billing16.proteingroups.txt')
inv <- c('EM_E', 'BM_E', 'BM_EM')
object <- read_proteingroups(
  file, invert_subgroups=inv, fit='limma', plot=FALSE)
dim(limma(object))
dim(limma(object[1:5, ]))
```

| | |
|------------|---------------------------|
| log2counts | <i>Get/Set log2counts</i> |
|------------|---------------------------|

Description

Get / Set log2counts matrix

Usage

```
log2counts(object)

## S4 method for signature 'SummarizedExperiment'
log2counts(object)

log2counts(object) <- value

## S4 replacement method for signature 'SummarizedExperiment,matrix'
log2counts(object) <- value

## S4 replacement method for signature 'SummarizedExperiment,numeric'
log2counts(object) <- value
```

Arguments

| | |
|--------|---------------------------------------|
| object | SummarizedExperiment |
| value | log2count matrix (features x samples) |

Value

log2count matrix (get) or updated object (set)

Examples

```
file <- download_data('billing19.rnacounts.txt')
object <- read_rnaseq_counts(file, plot=FALSE)
log2counts(object) <- values(object)
log2counts(object)[1:3, 1:3]
```

| | |
|------------------|---------------------------------|
| log2countsratios | <i>Get/Set log2countsratios</i> |
|------------------|---------------------------------|

Description

Get / Set log2countsratios matrix

Usage

```
log2countsratios(object)

## S4 method for signature 'SummarizedExperiment'
log2countsratios(object)

log2countsratios(object) <- value

## S4 replacement method for signature 'SummarizedExperiment,matrix'
log2countsratios(object) <- value

## S4 replacement method for signature 'SummarizedExperiment,numeric'
log2countsratios(object) <- value
```

Arguments

| | |
|--------|--|
| object | SummarizedExperiment |
| value | log2countsratios matrix (features x samples) |

Value

log2countsratios matrix (get) or updated object (set)

Examples

```
file <- download_data('billing19.rnacounts.txt')
object <- read_rnaseq_counts(file, plot=FALSE)
log2countsratios(object) <- values(object)
log2countsratios(object)[1:3, 1:3]
```

| | |
|---------|------------------------|
| log2cpm | <i>Get/Set log2cpm</i> |
|---------|------------------------|

Description

Get / Set log2cpm matrix

Usage

```
log2cpm(object)

## S4 method for signature 'SummarizedExperiment'
log2cpm(object)

log2cpm(object) <- value

## S4 replacement method for signature 'SummarizedExperiment,matrix'
log2cpm(object) <- value

## S4 replacement method for signature 'SummarizedExperiment,numeric'
log2cpm(object) <- value
```

Arguments

| | |
|--------|-------------------------------------|
| object | SummarizedExperiment |
| value | log2cpm matrix (features x samples) |

Value

log2cpm matrix (get) or updated object (set)

Examples

```
file <- download_data('billing19.rnacounts.txt')
object <- read_rnaseq_counts(file, plot=FALSE)
log2cpm(object) <- values(object)
log2cpm(object)[1:3, 1:3]
```

| | |
|---------------|------------------------------|
| log2cpmratios | <i>Get/Set log2cpmratios</i> |
|---------------|------------------------------|

Description

Get / Set log2cpmratios matrix

Usage

```
log2cpmratios(object)

## S4 method for signature 'SummarizedExperiment'
log2cpmratios(object)

log2cpmratios(object) <- value

## S4 replacement method for signature 'SummarizedExperiment,matrix'
log2cpmratios(object) <- value

## S4 replacement method for signature 'SummarizedExperiment,numeric'
log2cpmratios(object) <- value
```

Arguments

| | |
|--------|---|
| object | SummarizedExperiment |
| value | log2cpmratios matrix (features x samples) |

Value

log2cpmratios matrix (get) or updated object (set)

Examples

```
file <- download_data('billing19.rnacounts.txt')
object <- read_rnaseq_counts(file, plot=FALSE)
log2cpmratios(object) <- values(object)
log2cpmratios(object)[1:3, 1:3]
```

| | |
|---------|------------------------|
| log2tpm | <i>Get/Set log2tpm</i> |
|---------|------------------------|

Description

Get / Set log2tpm matrix

Usage

```
log2tpm(object)

## S4 method for signature 'SummarizedExperiment'
log2tpm(object)

log2tpm(object) <- value

## S4 replacement method for signature 'SummarizedExperiment,matrix'
log2tpm(object) <- value

## S4 replacement method for signature 'SummarizedExperiment,numeric'
log2tpm(object) <- value
```

Arguments

| | |
|--------|-------------------------------------|
| object | SummarizedExperiment |
| value | log2tpm matrix (features x samples) |

Value

log2tpm matrix (get) or updated object (set)

Examples

```
file <- download_data('billing19.rnacounts.txt')
object <- read_rnaseq_counts(file, plot=FALSE)
log2tpm(object) <- values(object)
log2tpm(object)[1:3, 1:3]
```

| | |
|---------------|------------------------------|
| log2tpmratios | <i>Get/Set log2tpmratios</i> |
|---------------|------------------------------|

Description

Get / Set log2tpmratios matrix

Usage

```
log2tpmratios(object)

## S4 method for signature 'SummarizedExperiment'
log2tpmratios(object)

log2tpmratios(object) <- value

## S4 replacement method for signature 'SummarizedExperiment,matrix'
log2tpmratios(object) <- value

## S4 replacement method for signature 'SummarizedExperiment,numeric'
log2tpmratios(object) <- value
```

Arguments

| | |
|--------|---|
| object | SummarizedExperiment |
| value | log2tpmratios matrix (features x samples) |

Value

log2tpmratios matrix (get) or updated object (set)

Examples

```
file <- download_data('billing19.rnacounts.txt')
object <- read_rnaseq_counts(file, plot=FALSE)
log2tpmratios(object) <- values(object)
log2tpmratios(object)[1:3, 1:3]
```

| | |
|---------------|-------------------------|
| log2transform | <i>Transform values</i> |
|---------------|-------------------------|

Description

Transform values

Usage

```
log2transform(object, verbose = FALSE)
exp2(object, verbose = FALSE)
zscore(object, verbose = FALSE)
quantnorm(object, verbose = FALSE)
invnorm(object, verbose = FALSE)
```

Arguments

| | |
|---------|----------------------|
| object | SummarizedExperiment |
| verbose | TRUE or FALSE |

Value

Transformed sumexp

Examples

```
require(magrittr)
file <- download_data('fukuda20.proteingroups.txt')
object <- read_proteingroups(file, plot=FALSE, impute=FALSE)

object %>% plot_sample_densities()
invnorm(object) %>% plot_sample_densities()

object %>% plot_sample_densities()
quantnorm(object) %>% plot_sample_densities()

object %>% plot_sample_densities()
zscore(object) %>% plot_sample_densities()

object %>% plot_sample_densities()
exp2(object) %>% plot_sample_densities()
log2transform(exp2(object)) %>% plot_sample_densities()
```

| | |
|-----------------|---------------------------------|
| make_volcano_dt | <i>Create volcano datatable</i> |
|-----------------|---------------------------------|

Description

Create volcano datatable

Usage

```
make_volcano_dt(  
  object,  
  fit,  
  contrastdefmat = contrastdefs(object)[[1]],  
  ntop = 3  
)
```

Arguments

| | |
|----------------|------------------------------------|
| object | SummarizedExperiment |
| fit | 'limma', 'lme', 'lm', 'wilcoxon' |
| contrastdefmat | contrastdef matrix |
| ntop | no of top features to be annotated |

Value

data.table

Examples

```
file <- download_data('fukuda20.proteingroups.txt')  
object <- read_proteingroups(file, fit='limma', plot=FALSE)  
make_volcano_dt(object, fit = 'limma')
```

| | |
|---------------|---|
| matrix2sumexp | <i>Convert matrix into SummarizedExperiment</i> |
|---------------|---|

Description

Convert matrix into SummarizedExperiment

Usage

```
matrix2sumexp(  
  x,  
  sdt = NULL,  
  sdtby = if (is.null(sdt)) NULL else names(sdt)[1],  
  subgroupvar = NULL,  
  fdt = NULL,  
  fdtby = if (is.null(fdt)) NULL else names(fdt)[1],  
  fnamevar = NULL,  
  verbose = TRUE  
)
```

Arguments

| | |
|-------------|---|
| x | matrix |
| sdt | sample data.table / data.frame / DataFrame |
| sdtby | sample data mergeby column |
| subgroupvar | string / NULL |
| fdt | feature data.table / data.frame / DataFrame |
| fdtby | feature data mergeby column |
| fnamevar | string / NULL |
| verbose | TRUE/FALSE |

Value

SummarizedExperiment

Examples

```
require(magrittr)  
file <- download_data('atkin18.metabolon.xlsx')  
x <- values(read_metabolon(file, plot=FALSE))  
object <- matrix2sumexp(x)  
object %<>% pca()  
biplot(object, nloadings=0, color=subgroup)
```

MAXQUANT_PATTERNS_PEP COUNTS

maxquant peptide count patterns

Description

maxquant peptide count patterns

Usage

MAXQUANT_PATTERNS_PEP COUNTS

Format

An object of class character of length 3.

Examples

MAXQUANT_PATTERNS_PEP COUNTS

MAXQUANT_PATTERNS_QUANTITY
maxquant quantity patterns

Description

maxquant quantity patterns

Usage

MAXQUANT_PATTERNS_QUANTITY

Format

An object of class character of length 7.

Examples

MAXQUANT_PATTERNS_QUANTITY

merge_sdata *Merge sample/feature data*

Description

Merge sample/feature data

Usage

```
merge_sdata(
  object,
  dt,
  by.x = "sample_id",
  by.y = names(dt)[1],
  verbose = TRUE
)

merge_fdata(
  object,
  dt,
  by.x = "feature_id",
  by.y = names(dt)[1],
  verbose = TRUE
)
```

Arguments

| | |
|---------|-----------------------------------|
| object | SummarizedExperiment |
| dt | data.frame, data.table, DataFrame |
| by.x | object mergevar |
| by.y | df mergevar |
| verbose | TRUE/FALSE |

Value

SummarizedExperiment

Examples

```
require(magrittr)
file <- download_data('halama18.metabolon.xlsx')
object <- read_metabolon(file, plot=FALSE)
object %<>% merge_sdata( data.frame(sample_id = object$sample_id,
                                   number = seq_along(object$sample_id)))
head(sdata(object))
```

merge_sfile

Merge sample/feature file

Description

Merge sample/feature file

Usage

```
merge_sfile(
  object,
  sfile = NULL,
  by.x = "sample_id",
  by.y = NULL,
  stringsAsFactors = TRUE,
  verbose = TRUE
)
```

```
merge_ffile(
  object,
  ffile = NULL,
  by.x = "feature_id",
  by.y = NULL,
  stringsAsFactors = TRUE,
  verbose = TRUE
)
```

Arguments

| | |
|------------------|-------------------------|
| object | SummarizedExperiment |
| sfile | sample file path |
| by.x | object mergevar |
| by.y | file mergevar |
| stringsAsFactors | TRUE or FALSE |
| verbose | TRUE (default) or FALSE |
| ffile | ffile path |

Value

SummarizedExperiment

Examples

```
require(magrittr)
file <- download_data('billing19.proteingroups.txt')
select <- c('E00','E01', 'E02','E05','E15','E30', 'M00')
select %<>% paste0('_STD')
object <- read_proteingroups(file, select_subgroups = select, plot=FALSE)
sfile <- paste0(tempdir(), '/', basename(tools::file_path_sans_ext(file)))
sfile %<>% paste0('.samples.txt')
invisible(create_sfile(object, sfile))
merge_sfile(object, sfile)
```

| | |
|------------|--------------------------|
| message_df | <i>message dataframe</i> |
|------------|--------------------------|

Description

message dataframe using sprintf syntax. Use place holder `

Usage

```
message_df(format_string, x)
```

Arguments

| | |
|---------------|-----------------------------|
| format_string | sprintf style format string |
| x | data.frame |

Value

nothing returned

Examples

```
x <- data.frame(feature_id = c('F001', 'F002'), symbol = c('FEAT1', 'FEAT2'))
message_df('\t%s', x)
```

```
x <- c(rep('PASS', 25), rep('FAIL', 25))
message_df(format_string = '%s', table(x))
```

| | |
|----------|-------------------------------|
| nfactors | <i>stri_split and extract</i> |
|----------|-------------------------------|

Description

stri_split and extract

Usage

```
nfactors(x, sep = guess_sep(x))
```

```
split_extract(x, i, sep = guess_sep(x))
```

Arguments

| | |
|-----|---------|
| x | string |
| sep | string |
| i | integer |

Value

character

Examples

```
require(magrittr)
file <- download_data('halama18.metabolon.xlsx')
object <- read_metabolon(file, plot=FALSE)
x <- object$sample_id[1:5]
nfactors(x)
split_extract(x, 1:2)
split_extract(x, seq_len(nfactors(x)-1))
split_extract(x, nfactors(x))

# With NA values
split_extract(fdata(object)$PUBCHEM, 1, ';')
```

normimpute

Impute from half-normal distribution around 0

Description

Impute from half-normal distribution around 0

Usage

```
normimpute(x, selector = is.na(x), mean = 0)
```

```
halfnormimpute(x, selector = is.na(x))
```

```
zeroimpute(x, selector = is.na(x))
```

```
translate(
  x,
  ref = c(min, mean, median, max)[[1]],
  pos = 3 * sd(x, na.rm = TRUE)
)
```

Arguments

| | |
|----------|---|
| x | NA-containing numeric vector |
| selector | which values to impute |
| mean | number |
| ref | reference : which reference value away from which to impute |
| pos | position : how many sds away to impute |

Value

numeric vector of same length

Examples

```
require(data.table)
x <- rnorm(1e5)
idx <- runif(length(x))>0.9
x[idx] <- NA
dt1 <- data.table(value = normimpute(x), distr = 'norm')

x <- abs(rnorm(1e5)); x[idx] <- NA
dt2 <- data.table(value = halfnormimpute(x), distr = 'halfnorm')

x <- abs(rnorm(1e5)); x[idx] <- NA
dt3 <- data.table(value = zeroimpute(x), distr = 'zero')

x <- abs(rnorm(1e5)); x[idx] <- NA
dt4 <- data.table(value = translate(x), distr = 'translate')

require(ggplot2)
ggplot(rbind(dt1,dt2,dt3, dt4), aes(x=value, fill=distr)) +
  geom_density(alpha=0.5)
```

occupancies

Get/Set occupancies

Description

Get / Set phosphosite occupancies matrix

Usage

```
occupancies(object)

## S4 method for signature 'SummarizedExperiment'
occupancies(object)

occupancies(object) <- value

## S4 replacement method for signature 'SummarizedExperiment,matrix'
occupancies(object) <- value

## S4 replacement method for signature 'SummarizedExperiment,numeric'
occupancies(object) <- value
```

Arguments

object SummarizedExperiment
value occupancy matrix (features x samples)

Value

occupancy matrix (get) or updated object (set)

Examples

```
file <- download_data('fukuda20.proteingroups.txt')  
object <- read_proteingroups(file, plot=FALSE)  
occupancies(object)  
occupancies(object) <- values(object)  
occupancies(object)[1:3, 1:3]
```

pca

Add PCA, SMA, LDA, PLS

Description

Perform a dimension reduction. Add sample scores, feature loadings, and dimension variances to object.

Usage

```
pca(object, ndim = 2, minvar = 0, verbose = TRUE, plot = FALSE, ...)
```

```
pls(  
  object,  
  subgroupvar = "subgroup",  
  ndim = 2,  
  minvar = 0,  
  verbose = FALSE,  
  plot = FALSE,  
  ...  
)
```

```
sma(object, ndim = 2, minvar = 0, verbose = TRUE, plot = FALSE, ...)
```

```
lda(  
  object,  
  subgroupvar = "subgroup",  
  ndim = 2,  
  minvar = 0,  
  verbose = TRUE,  
  plot = FALSE,
```

```
    ...
  )
```

Arguments

| | |
|-------------|-------------------------|
| object | SummarizedExperiment |
| ndim | number |
| minvar | number |
| verbose | TRUE (default) or FALSE |
| plot | TRUE/FALSE |
| ... | passed to biplot |
| subgroupvar | subgroup svar |

Value

SummarizedExperiment

Author(s)

Aditya Bhagwat, Laure Cougnaud (LDA)

Examples

```
file <- download_data('atkin18.metabolon.xlsx')
object <- read_metabolon(file, plot = FALSE)
pca(object, plot=TRUE, color = Group) # Principal Component Analysis
pls(object, subgroupvar = 'Group') # Partial Least Squares
lda(object, subgroupvar = 'Group') # Linear Discriminant Analysis
sma(object) # Spectral Map Analysis
pca(object, ndim=3)
pca(object, ndim=Inf, minvar=5)
```

plot_boxplots

Plot sample/feature boxplots

Description

Plot sample/feature boxplots

Usage

```
plot_boxplots(
  object,
  x,
  fill,
  color = NULL,
  facet = NULL,
```

```
    highlight = NULL,  
    fixed = list(na.rm = TRUE)  
  )  
  
plot_sample_boxplots(  
  object,  
  x = sample_id,  
  fill = sample_id,  
  color = NULL,  
  highlight = NULL,  
  fixed = list(na.rm = TRUE)  
)  
  
plot_feature_boxplots(  
  object,  
  x = feature_id,  
  fill = feature_id,  
  color = NULL,  
  highlight = NULL,  
  fixed = list(na.rm = TRUE)  
)  
  
plot_subgroup_boxplots(  
  object,  
  subgroup,  
  x = !!enquo(subgroup),  
  fill = !!enquo(subgroup),  
  color = NULL,  
  highlight = NULL,  
  facet = feature_id,  
  fixed = list(na.rm = TRUE)  
)
```

Arguments

| | |
|-----------|---|
| object | SummarizedExperiment |
| x | svar mapped to x |
| fill | svar mapped to fill |
| color | svar mapped to color |
| facet | svar mapped to facet |
| highlight | fvar expressing which feature should be highlighted |
| fixed | fixed aesthetics |
| subgroup | subgroup svar symbol |

Value

ggplot object

See Also

[plot_sample_densities](#), [plot_sample_violins](#)

Examples

```
# data
require(magrittr)
file <- download_data('halama18.metabolon.xlsx')
object <- read_metabolon(file, plot = FALSE)
object %<>% extract(, order(.$Group))
fdata(object) %<>% cbind(
  control=.$feature_name %in% c('biotin','phosphate'))

# plot
plot_boxplots(object[1:9,], x = feature_id, fill = feature_id)
plot_boxplots(object[,1:9], x = sample_id, fill = sample_id )
plot_feature_boxplots(object[1:9, ])
plot_sample_boxplots(object[, 1:12])
plot_sample_boxplots(object[, 1:12], highlight = control)
plot_subgroup_boxplots(object[1:2, ], subgroup = Group)
```

plot_contrastogram *Plot contrastogram*

Description

Plot contrastogram

Usage

```
plot_contrastogram(
  object,
  subgroupvar,
  formula = default_formula(object, subgroupvar, "limma"),
  colors = make_colors(slevels(object, subgroupvar), guess_sep(object)),
  curve = 0.1
)
```

Arguments

| | |
|-------------|--|
| object | SummarizedExperiment |
| subgroupvar | subgroup svar |
| formula | formula |
| colors | named color vector (names = subgroups) |
| curve | arrow curvature |

Value

list returned by [plotmat](#)

Examples

```

if (requireNamespace('diagram', quietly = TRUE)){
  file <- download_data('halama18.metabolon.xlsx')
  object <- read_metabolon(file, fit='limma', plot=FALSE)
  plot_contrastogram(object, subgroupvar = 'Group')
}

```

plot_corrections *Biplot batch corrections*

Description

Biplot batch corrections

Usage

```
plot_corrections(...)
```

```

biplot_corrections(
  object,
  method = "pca",
  color = subgroup,
  covariates = character(0),
  varcols = ceiling(sqrt(1 + length(covariates))),
  plot = TRUE
)

```

Arguments

| | |
|------------|---------------------------------------|
| ... | used to maintain deprecated functions |
| object | SummarizedExperiment |
| method | 'pca', 'pls', 'lda', or 'sma' |
| color | variable mapped to color (symbol) |
| covariates | covariates to be batch-corrected |
| varcols | number of covariate columns |
| plot | TRUE/FALSE: plot? |

Value

grid object

See Also

biplot_covariates

Examples

```
file <- download_data('atkin18.metabolon.xlsx')
object <- read_metabolon(file, pca=TRUE, plot = FALSE)
biplot_corrections(
  object, color = Group, covariates = c('SEX', 'T2D', 'SUB', 'SET'))
```

| | |
|-----------------|--------------------------|
| plot_covariates | <i>Biplot covariates</i> |
|-----------------|--------------------------|

Description

Biplot covariates

Usage

```
plot_covariates(...)

biplot_covariates(
  object,
  method = "pca",
  covariates = "subgroup",
  ndim = 6,
  dimcols = 1,
  varcols = length(covariates),
  plot = TRUE
)
```

Arguments

| | |
|------------|--|
| ... | used to maintain deprecated functions |
| object | SummarizedExperiment |
| method | 'pca', 'pls', 'lda', or 'sma' |
| covariates | covariates: mapped to color or batch-corrected |
| ndim | number of dimensions to plot |
| dimcols | number of dimension columns |
| varcols | number of covariate columns |
| plot | TRUE or FALSE: whether to plot |

Value

ggplot object

See Also

biplot_corrections

Examples

```

file <- download_data('atkin18.metabolon.xlsx')
object <- read_metabolon(file, pca = TRUE, plot = FALSE)
biplot_covariates(object, covariates = 'Group', ndim = 12, dimcols = 3)
biplot_covariates(object, covariates = c('SEX', 'T2D', 'SUB', 'SET'))
biplot_covariates(object, covariates = c('SEX', 'T2D', 'SUB', 'SET'), ndim=2)
biplot_covariates(object, covariates = c('Group'), dimcols = 3)

```

plot_data

Plot data

Description

Plot data

Usage

```

plot_data(
  data,
  geom = geom_point,
  color = NULL,
  fill = !!enquo(color),
  ...,
  fixed = list(),
  theme = list()
)

```

Arguments

| | |
|-------|---------------------------------------|
| data | data.frame' |
| geom | geom_point, etc. |
| color | variable mapped to color (symbol) |
| fill | variable mapped to fill (symbol) |
| ... | mapped aesthetics |
| fixed | fixed aesthetics (list) |
| theme | list with ggplot theme specifications |

Value

ggplot object

Author(s)

Aditya Bhagwat, Johannes Graumann

Examples

```

require(magrittr)
file <- download_data('halama18.metabolon.xlsx')
object <- read_metabolon(file, plot = FALSE)
object %<>% pca()
data <- sdata(object)
plot_data(data, x = pca1, y = pca2)
plot_data(data, x = pca1, y = pca2, color = TIME_POINT)
data$TIME <- as.numeric(substr(data$TIME_POINT, 2, 3))
plot_data(data, x = pca1, y = pca2, color = TIME)
plot_data(data, x = pca1, y = pca2, color = NULL)

fixed <- list(shape = 15, size = 3)
plot_data(data, x = pca1, y = pca2, fixed=fixed)

```

plot_densities

Plot sample/feature densities

Description

Plot sample/feature densities

Usage

```

plot_densities(
  object,
  group,
  fill,
  color = NULL,
  fixed = list(alpha = 0.5, na.rm = TRUE)
)

plot_sample_densities(
  object,
  fill = sample_id,
  color = NULL,
  group = sample_id,
  fixed = list(alpha = 0.5, na.rm = TRUE),
  subsetter = if (ncol(object) < 100) {
    seq_len(ncol(object))
  } else {
    sample(ncol(object), 9)
  }
)

plot_feature_densities(

```

```
object,  
fill = feature_id,  
color = NULL,  
group = feature_id,  
fixed = list(alpha = 0.5, na.rm = TRUE),  
subsetter = if (nrow(object) < 100) {  
  seq_len(nrow(object))  
} else {  
  sample(nrow(object), 9)  
}  
)
```

Arguments

| | |
|-----------|--|
| object | SummarizedExperiment |
| group | svar mapped to group |
| fill | svar mapped to fill |
| color | svar mapped to color |
| fixed | fixed aesthetics |
| subsetter | subsetter for showing a subset of samples/features |

Value

ggplot object

See Also

[plot_sample_violins](#), [plot_sample_boxplots](#)

Examples

```
# Read data  
require(magrittr)  
file <- download_data('atkin18.metabolon.xlsx')  
object <- read_metabolon(file, plot = FALSE)  
object %<>% extract(, order(.$Group))  
# Plot distributions  
plot_sample_densities(object, fill = Group)  
plot_feature_densities(object)
```

| | |
|--------------|------------------------|
| plot_detects | <i>Plot detections</i> |
|--------------|------------------------|

Description

Plot detections

Usage

```
plot_detects(...)  
  
plot_detections(object, subgroup = subgroup, fill = !!enquo(subgroup))  
  
plot_quantifications(...)  
  
plot_summarized_detections(  
  object,  
  subgroup = subgroup,  
  fill = !!enquo(subgroup),  
  na_imputes = TRUE  
)
```

Arguments

| | |
|------------|--|
| ... | for backward compatilby |
| object | SummarizedExperiment |
| subgroup | subgroup var (sym) |
| fill | fill var (sym) |
| na_imputes | whether to NA imputes prior to plottin (TRUE/FALSE)g |

Details

`plot_detections` plots feature x sample detections. It shows per feature/sample nondetects (white), imputes (light colored), and detects (full color).

`plot_summarized_detections` gives an summarized view, plotting featuretype x subgroup detections. It visualizes the subgroup-wise nondetect structure often seen in mass spectrometry proteomics data (across e.g. different cell types)

Value

ggplot object

Examples

```

require(magrittr)
file <- download_data('fukuda20.proteingroups.txt')
object <- read_proteingroups(file, impute=FALSE, plot = FALSE)
plot_summarized_detections(object)
plot_detections(object)
plot_detections(impute_systematic_nondetects(object, plot=FALSE))

file <- download_data('halama18.metabolon.xlsx')
object <- read_metabolon(file, impute = FALSE, plot = FALSE)
plot_summarized_detections(object, Group)
plot_detections(object, Group)

```

plot_features

Plot features

Description

Plot features

Usage

```

plot_features(
  object,
  geom,
  subgroup,
  x = !!enquo(subgroup),
  fill = !!enquo(subgroup),
  color = !!enquo(subgroup),
  ...,
  fixed = list(na.rm = TRUE),
  theme = list(axis.text.x = element_blank(), axis.title.x = element_blank(),
    axis.ticks.x = element_blank())
)

plot_feature_profiles(...)

```

Arguments

| | |
|----------|--------------------------------|
| object | SummarizedExperiment |
| geom | geom_point, geom_boxplot, etc. |
| subgroup | subgroup svar |
| x | svar mapped to x |
| fill | svar mapped to fill |
| color | svar mapped to color |
| ... | mapped aesthetics |

fixed fixed aesthetics
 theme ggplot theme specifications

Value

ggplot object

Examples

```
require(magrittr)
file <- download_data('halama18.metabolon.xlsx')
object <- read_metabolon(file, pca=TRUE, plot = FALSE)
idx <- order(abs(fdata(object)$pca1), decreasing=TRUE)[1:9]
object %<>% extract(idx, )
plot_feature_boxplots(object)
plot_subgroup_boxplots(object, subgroup=Group)
plot_feature_profiles( object, subgroup=Group)
```

| | |
|-----------|------------------|
| plot_venn | <i>Plot venn</i> |
|-----------|------------------|

Description

Plot venn

Usage

```
plot_venn(isfdr)
```

Arguments

isfdr matrix(nrow, ncontrast): -1 (down), +1 (up)

Value

nothing returned

Examples

```
require(magrittr)
file <- download_data('atkin18.somascan.adat')
object <- read_somascan(file, plot=FALSE)
object %<>% fit_wilcoxon(subgroupvar='SampleGroup', block = 'Subject_ID')
object %<>% fit_limma( subgroupvar='SampleGroup', block = 'Subject_ID')
isfdr <- is_sig(object, contrast = 't3-t2')
plot_venn(isfdr)
```

| | |
|--------------|------------------------------------|
| plot_violins | <i>Plot sample/feature violins</i> |
|--------------|------------------------------------|

Description

Plot sample/feature violins

Usage

```
plot_violins(  
  object,  
  x,  
  fill,  
  color = NULL,  
  group = NULL,  
  facet = NULL,  
  highlight = NULL,  
  fixed = list(na.rm = TRUE)  
)
```

```
plot_sample_violins(  
  object,  
  x = sample_id,  
  fill = sample_id,  
  color = NULL,  
  highlight = NULL,  
  fixed = list(na.rm = TRUE)  
)
```

```
plot_feature_violins(  
  object,  
  x = feature_id,  
  fill = feature_name,  
  color = NULL,  
  highlight = NULL,  
  fixed = list(na.rm = TRUE)  
)
```

```
plot_subgroup_violins(  
  object,  
  subgroup,  
  x = !!enquo(subgroup),  
  fill = !!enquo(subgroup),  
  color = NULL,  
  highlight = NULL,  
  facet = feature_id,  
  fixed = list(na.rm = TRUE)
```


)

Arguments

| | |
|-----------|---|
| object | SummarizedExperiment |
| x | svar mapped to x |
| fill | svar mapped to fill |
| color | svar mapped to color |
| group | svar mapped to group |
| facet | svar mapped to facets |
| highlight | fvar expressing which feature should be highlighted |
| fixed | fixed aesthetics |
| subgroup | subgroup svar |

Value

ggplot object

See Also[plot_sample_densities](#), [plot_sample_boxplots](#)**Examples**

```
# data
require(magrittr)
file <- download_data('halama18.metabolon.xlsx')
object <- read_metabolon(file, plot = FALSE)
object %<>% extract(, order(.$Group))
control_features <- c('biotin', 'phosphate')
fdata(object) %<>% cbind(control=.$feature_name %in% control_features)

# plot
plot_violins(object[1:12, ], x=feature_id, fill=feature_id)
plot_feature_violins(object[1:12, ])
plot_sample_violins(object[, 1:12], highlight = control)
plot_subgroup_violins(object[1:4, ], subgroup = Group)
```

`plot_volcano`*Plot volcano*

Description

Plot volcano

Usage

```
plot_volcano(
  object,
  fit = intersect(names(metadata(object)), TESTS)[1],
  contrastdefs = autonomics::contrastdefs(object)[[1]],
  label = feature_name,
  ntop = 1
)
```

Arguments

| | |
|--------------|--|
| object | SummarizedExperiment |
| fit | 'limma', 'lme', 'lm', 'wilcoxon' |
| contrastdefs | contrastdef vector / matrix / list |
| label | fvar for labeling top features |
| ntop | number: n top features to be annotated |

Value

ggplot object

Examples

```
file <- download_data('fukuda20.proteingroups.txt')
object <- read_proteingroups(file, fit='limma', plot=FALSE)
plot_volcano(object)
```

```
preprocess_rnaseq_counts
```

Preprocess RNAseq counts

Description

Preprocess RNAseq counts

Usage

```
preprocess_rnaseq_counts(
  object,
  subgroupvar = if ("subgroup" %in% svars(object)) "subgroup" else NULL,
  formula = default_formula(object, subgroupvar, "limma"),
  block = NULL,
  min_count = 10,
  pseudocount = 0.5,
  genesize = NULL,
  cpm = TRUE,
```

```
tmm = cpm,
voom = TRUE,
log2 = TRUE,
verbose = TRUE,
plot = TRUE
)
```

Arguments

| | |
|-------------|--|
| object | SummarizedExperiment |
| subgroupvar | subgroup svar |
| formula | designmat formula |
| block | block svar |
| min_count | min count required in some samples |
| pseudocount | added pseudocount to avoid log(x)=-Inf |
| genesize | genesize fvar to compute tpm |
| cpm | whether to compute counts per million (scaled) reads |
| tmm | whether to tmm normalize |
| voom | whether to voom weight |
| log2 | whether to log2 |
| verbose | whether to msg |
| plot | whether to plot |

Value

SummarizedExperiment

Examples

```
require(magrittr)
file <- download_data('billing19.rnacounts.txt')
object <- .read_rnaseq_counts(file)
object$subgroup
object %<>% preprocess_rnaseq_counts()
```

| | |
|---------------|------------------------------|
| proteingroups | <i>Get/Set proteingroups</i> |
|---------------|------------------------------|

Description

Get / Set proteingroups matrix

Usage

```

proteingroups(object)

## S4 method for signature 'SummarizedExperiment'
proteingroups(object)

proteingroups(object) <- value

## S4 replacement method for signature 'SummarizedExperiment,matrix'
proteingroups(object) <- value

## S4 replacement method for signature 'SummarizedExperiment,numeric'
proteingroups(object) <- value

```

Arguments

| | |
|--------|---------------------------------------|
| object | SummarizedExperiment |
| value | occupancy matrix (features x samples) |

Value

occupancy matrix (get) or updated object (set)

Examples

```

file <- download_data('fukuda20.proteingroups.txt')
object <- read_proteingroups(file, plot=FALSE)
proteingroups(object)[1:3, 1:3]

```

| | |
|-----------------|-----------------------------------|
| read_affymetrix | <i>Read affymetrix microarray</i> |
|-----------------|-----------------------------------|

Description

Read affymetrix microarray

Usage

```
read_affymetrix(celfiles)
```

Arguments

| | |
|----------|-------------------------------|
| celfiles | string vector: CEL file paths |
|----------|-------------------------------|

Value

RangedSummarizedExperiment

Examples

```

require(magrittr)
url <- paste0('http://www.bioconductor.org/help/publications/2003/',
             'Chiaretti/chiaretti2/T33.tgz')
localdir <- file.path(rappdirs::user_cache_dir(appname = 'autonomics'), 'T33')
dir.create(localdir, showWarnings=FALSE)
localfile <- file.path(localdir, basename(url))
if (!file.exists(localfile)){
  download.file(url, destfile = localfile)
  untar(localfile, exdir = path.expand(localdir))
}
localfile %<>% substr(1, nchar(.)-4)
if (!requireNamespace("BiocManager", quietly = TRUE)) install.packages(
  'BiocManager')
if (!requireNamespace("hgu95av2.db", quietly = TRUE)) BiocManager::install(
  'hgu95av2.db')
# read_affymetrix(cefiles = list.files(localfile, full.names = TRUE))
# currently openblas issue: https://stackoverflow.com/questions/61629861/

```

rm_singleton_samples *Rm singleton samples*

Description

Rm singleton samples

Usage

```
rm_singleton_samples(object, svar = "subgroup", verbose = TRUE)
```

Arguments

| | |
|---------|----------------------|
| object | SummarizedExperiment |
| svar | sample var |
| verbose | TRUE/FALSE |

Value

SummarizedExperiment

Examples

```

require(magrittr)
file <- download_data('atkin18.somascan.adat')
object <- read_somascan(file, plot=FALSE)
object %<>% filter_samples(SampleGroup %in% c('t1', 't2'), verbose = TRUE)
rm_singleton_samples(object, 'Subject_ID')

```

| | |
|----------------|--------------------------------|
| scaledlibsizes | <i>Get tmm-scaled libsizes</i> |
|----------------|--------------------------------|

Description

Get tmm-scaled libsizes

Usage

```
scaledlibsizes(counts)
```

Arguments

counts counts matrix

Value

scaled libsize vector

Examples

```
file <- download_data('billing19.rnacounts.txt')
object <- read_rnaseq_counts(file, cpm=FALSE, log2=FALSE, plot=FALSE)
scaledlibsizes(counts(object))
```

| | |
|-------|----------------------|
| sdata | <i>Get/Set sdata</i> |
|-------|----------------------|

Description

Get/Set sample data

Usage

```
sdata(object)

## S4 method for signature 'SummarizedExperiment'
sdata(object)

## S4 method for signature 'MultiAssayExperiment'
sdata(object)

sdata(object) <- value

## S4 replacement method for signature 'SummarizedExperiment,data.frame'
sdata(object) <- value
```

```
## S4 replacement method for signature 'SummarizedExperiment,DataFrame'
sdata(object) <- value

## S4 replacement method for signature 'MultiAssayExperiment,data.frame'
sdata(object) <- value

## S4 replacement method for signature 'MultiAssayExperiment,DataFrame'
sdata(object) <- value
```

Arguments

| | |
|--------|--------------------------------------|
| object | SummarizedExperiment, eSet, or EList |
| value | dataframe |

Value

sample dataframe (get) or updated object (set)

Examples

```
require(magrittr)
file <- download_data('billing16.proteingroups.txt')
object <- read_proteingroups(file, plot=FALSE)
head(sdata(object))
head(sdata(object) %<>% cbind(z=1))
```

slevels

Get slevels

Description

Get svar levels

Usage

```
slevels(object, svar)

subgroup_levels(object)
```

Arguments

| | |
|--------|--------------------------------------|
| object | SummarizedExperiment, eSet, or eList |
| svar | sample var (character) |

Value

svar values (character)

Examples

```
file <- download_data('billing16.proteingroups.txt')
object <- read_proteingroups(file, plot=FALSE)
slevels(object, 'subgroup')
subgroup_levels(object)
```

snames

Get/Set snames

Description

Get/Set sample names

Usage

```
snames(object)

## S4 method for signature 'SummarizedExperiment'
snames(object)

snames(object) <- value

## S4 replacement method for signature 'SummarizedExperiment,character'
snames(object) <- value
```

Arguments

| | |
|--------|---------------------------------|
| object | SummarizedExperiment |
| value | string vector with sample names |

Value

sample names vector (get) or updated eSet (set)

Examples

```
require(magrittr)
file <- download_data('billing16.proteingroups.txt')
object <- read_proteingroups(file, plot=FALSE)
head(snames(object))
head(snames(object) %<>% paste0('SAMPLE_', .))
```

| | |
|---------------|----------------------|
| split_by_svar | <i>Split by svar</i> |
|---------------|----------------------|

Description

Split by svar

Usage

```
split_by_svar(object, svar = subgroup)
```

Arguments

| | |
|--------|----------------------|
| object | SummarizedExperiment |
| svar | svar to split on |

Value

list of SummarizedExperiment

Examples

```
file <- download_data('fukuda20.proteingroups.txt')
object <- read_proteingroups(file, impute=FALSE, plot = FALSE)
split_by_svar(object)
```

| | |
|-----------------------------|------------------------------------|
| standardize_maxquant_snames | <i>Standardize maxquant snames</i> |
|-----------------------------|------------------------------------|

Description

Standardize maxquant sample names

Usage

```
standardize_maxquant_snames(x, ...)

## S3 method for class 'character'
standardize_maxquant_snames(
  x,
  quantity = guess_maxquant_quantity(x),
  verbose = FALSE,
  ...
)
```

```
## S3 method for class 'SummarizedExperiment'
standardize_maxquant_snames(
  x,
  quantity = guess_maxquant_quantity(x),
  verbose = FALSE,
  ...
)
```

Arguments

| | |
|----------|--|
| x | character vector or SummarizedExperiment |
| ... | allow for proper S3 method dispatch |
| quantity | maxquant quantity |
| verbose | TRUE (default) or FALSE |

Details

Drop "Ratio normalized", "LFQ intensity" etc from maxquant sample names

Value

character vector or SummarizedExperiment

Examples

```
# character vector
x <- "Ratio M/L normalized STD(L)_E00(M)_E01(H)_R1"
standardize_maxquant_snames(x)

x <- "Ratio M/L STD(L)_E00(M)_E01(H)_R1"
standardize_maxquant_snames(x)

x <- 'LFQ intensity STD_R1'
standardize_maxquant_snames(x)

x <- 'LFQ intensity L STD(L)_E00(M)_E01(H)_R1'
standardize_maxquant_snames(x)

x <- 'Reporter intensity 0 A(0)_B(1)_C(2)_D(3)_E(4)_F(5)_R1'
standardize_maxquant_snames(x)

x <- 'Reporter intensity corrected 0 A(0)_B(1)_C(2)_D(3)_E(4)_F(5)_R1'
standardize_maxquant_snames(x)
```

| | |
|----------------|----------------------------|
| subgroup_array | <i>Get subgroup matrix</i> |
|----------------|----------------------------|

Description

Arrange (subgroup)levels in matrix

Usage

```
subgroup_array(object, subgroupvar)
subgroup_matrix(object, subgroupvar)
```

Arguments

| | |
|-------------|----------------------|
| object | SummarizedExperiment |
| subgroupvar | subgroup svar |

Value

matrix

Examples

```
file <- download_data('halama18.metabolon.xlsx')
object <- read_metabolon(file, plot=FALSE)
subgroup_matrix(object, 'Group')
```

| | |
|-------------------|--------------------------|
| subtract_baseline | <i>Subtract baseline</i> |
|-------------------|--------------------------|

Description

Subtract baseline level within block

Usage

```
subtract_baseline(
  object,
  subgroupvar,
  subgroupctr = slevels(object, subgroupvar)[1],
  block = NULL,
  assaynames = setdiff(assayNames(object), "weights"),
  verbose = TRUE
)
```

```

subtract_pairs(
  object,
  subgroupvar,
  subgroupctr = slevels(object, subgroupvar)[1],
  block,
  assaynames = setdiff(assayNames(object), "weights"),
  verbose = TRUE
)

subtract_differences(object, block, subgroupvar, verbose = TRUE)

```

Arguments

| | |
|-------------|--|
| object | SummarizedExperiment |
| subgroupvar | subgroup svar |
| subgroupctr | control subgroup |
| block | block svar (within which subtraction is performed) |
| assaynames | which assays to subtract for |
| verbose | TRUE/FALSE |

Details

subtract_baseline subtracts baseline levels within block, using the medoid baseline sample if multiple exist.

subtract_pairs also subtracts baseline level within block. It cannot handle multiple baseline samples, but has instead been optimized for many blocks

subtract_differences subtracts differences between subsequent levels, again within block

Value

SummarizedExperiment

Examples

```

# read
require(magrittr)
file <- download_data('atkin18.metabolon.xlsx')
object0 <- read_metabolon(file, plot=FALSE)
pca(object0, plot=TRUE, color=SET)

# subtract_baseline: takes medoid of baseline samples if multiple
object <- subtract_baseline(object0, block='SUB', subgroupvar='SET')
pca(object, plot=TRUE, color=SET)

# subtract_pairs: optimized for many blocks
object <- subtract_pairs( object0, block='SUB', subgroupvar='SET')

```

```
pca(object, plot=TRUE, color=SET)

# subtract differences
object <- subtract_differences(object0, block='SUB', subgroupvar='SET')
values(object) %<>% na_to_zero()
pca(object, plot=TRUE, color=SET)
```

sumexp2mae

Create MultiAssayExperiment from SummarizedExperiment list

Description

Create MultiAssayExperiment from SummarizedExperiment list

Usage

```
sumexp2mae(experiments)
```

Arguments

experiments named list of SummarizedExperiments

Value

MultiAssayExperiment

Examples

```
require(magrittr)
somascanfile <- download_data('atkin18.somascan.adat')
metabolonfile <- download_data('atkin18.metabolon.xlsx')
somascan <- read_somascan(somascanfile, plot=FALSE)
metabolon <- read_metabolon(metabolonfile, plot=FALSE)
svars(somascan) %<>% stringi::stri_replace_first_fixed(
  'SampleGroup', 'subgroup')
svars(metabolon) %<>% stringi::stri_replace_first_fixed(
  'Group', 'subgroup')
metabolon$replicate <- NULL
object <- sumexp2mae(list(somascan=somascan, metabolon=metabolon))
```

sumexp_to_wide_dt *Convert SummarizedExperiment into data.table*

Description

Convert SummarizedExperiment into data.table

Usage

```
sumexp_to_wide_dt(
  object,
  fid = "feature_id",
  fvars = intersect("feature_name", autonomics::fvars(object)),
  assay = assayNames(object)[1]
)

sumexp_to_long_dt(
  object,
  fid = "feature_id",
  fvars = intersect("feature_name", autonomics::fvars(object)),
  sid = "sample_id",
  svars = intersect("subgroup", autonomics::svars(object)),
  assay = assayNames(object) %>% intersect(c(.[1], "is_imputed"))
)

sumexp_to_subrep_dt(object, subgroup = subgroup)
```

Arguments

| | |
|----------|--------------------------------------|
| object | sumexp |
| fid | fvar carrying feature id |
| fvars | additional fvars to include in table |
| assay | matrix in assays(object) to be used |
| sid | svar carrying sample id |
| svars | additional svars to include in table |
| subgroup | subgroup (sym) |

Details

- sumexp_to_wide_dt: feature x sample
- sumexp_to_subrep_dt: feature.subgroup x replicate
- sumexp_to_long_dt: feature.sample

Value

data.table

Examples

```

# Stem cell comparison
file <- download_data('billing16.proteingroups.txt')
invert_subgroups <- c('EM_E', 'BM_E', 'EM_BM')
object <- read_proteingroups(file, invert_subgroups = invert_subgroups,
                             plot=FALSE)
sumexp_to_wide_dt(object)
sumexp_to_long_dt(object)
sumexp_to_subrep_dt(object)

# Glutaminase
require(magrittr)
file <- download_data('atkin18.metabolon.xlsx')
object <- read_metabolon(file, plot=FALSE)
sumexp_to_wide_dt(object)
sumexp_to_long_dt(object)
sumexp_to_subrep_dt(object, Group)

# Fukuda
require(magrittr)
file <- download_data('fukuda20.proteingroups.txt')
object <- read_proteingroups(file, impute=FALSE, plot=FALSE)
sumexp_to_long_dt(object)
object %<>% impute_systematic_nondetects(plot=FALSE)
sumexp_to_long_dt(object)

```

summarize_fit

Summarize fit

Description

Summarize fit

Usage

```
summarize_fit(object, fit = intersect(names(metadata(object)), TESTS)[1])
```

Arguments

| | |
|--------|---|
| object | SummarizedExperiment |
| fit | 'limma', 'lme', 'lm', 'lme', 'wilcoxon' |

Value

data.table(contrast, nup, ndown)

Examples

```
file <- download_data('billing19.rnacounts.txt')
object <- read_rnaseq_counts(file, fit='limma', plot=FALSE)
summarize_fit(object, 'limma')
```

svalues

Get/Set svalues

Description

Get/Set svar values

Usage

```
svalues(object, svar)
```

```
subgroup_values(object)
```

```
sampleid_values(object)
```

```
svalues(object, svar) <- value
```

```
## S4 replacement method for signature 'SummarizedExperiment,character'
svalues(object, svar) <- value
```

Arguments

object SummarizedExperiment

svar sample var (character)

value value vector

Value

character vector (get) or SummarizedExperiment (set)

Examples

```
file <- download_data('billing16.proteingroups.txt')
object <- read_proteingroups(file, plot=FALSE)
svalues(object, 'subgroup')
subgroup_values(object)
```

| | |
|-------|----------------------|
| svars | <i>Get/Set svars</i> |
|-------|----------------------|

Description

Get/Set sample variables

Usage

```
svars(object)

## S4 method for signature 'SummarizedExperiment'
svars(object)

## S4 method for signature 'MultiAssayExperiment'
svars(object)

svars(object) <- value

## S4 replacement method for signature 'SummarizedExperiment,character'
svars(object) <- value

## S4 replacement method for signature 'MultiAssayExperiment,character'
svars(object) <- value
```

Arguments

| | |
|--------|-----------------------------------|
| object | SummarizedExperiment |
| value | string factor with variable names |

Value

sample variable names (get) or updated SummarizedExperiment

Examples

```
require(magrittr)
file <- download_data('billing16.proteingroups.txt')
object <- read_proteingroups(file, plot=FALSE)
svars(object)[1]
(svars(object)[1] %<>% paste0('1'))
```

| | |
|-------|---|
| TESTS | <i>Statistical models supported in autonomics</i> |
|-------|---|

Description

Statistical models supported in autonomics

Usage

TESTS

Format

An object of class character of length 5.

Examples

TESTS

| | |
|-----|--------------------|
| tpm | <i>Get/Set tpm</i> |
|-----|--------------------|

Description

Get / Set tpm matrix

Usage

```
tpm(object)
```

```
## S4 method for signature 'SummarizedExperiment'  
tpm(object)
```

```
tpm(object) <- value
```

```
## S4 replacement method for signature 'SummarizedExperiment,matrix'  
tpm(object) <- value
```

```
## S4 replacement method for signature 'SummarizedExperiment,numeric'  
tpm(object) <- value
```

Arguments

| | |
|--------|---------------------------------|
| object | SummarizedExperiment |
| value | tpm matrix (features x samples) |

Value

tpm matrix (get) or updated object (set)

Examples

```
file <- download_data('billing19.rnacounts.txt')
object <- read_rnaseq_counts(file, plot=FALSE)
tpm(object) <- values(object)
tpm(object)[1:3, 1:3]
```

values

Get/Set expr values

Description

Get/Set value matrix

Usage

```
values(object)

## S4 method for signature 'SummarizedExperiment'
values(object)

values(object) <- value

## S4 replacement method for signature 'SummarizedExperiment,matrix'
values(object) <- value

## S4 replacement method for signature 'SummarizedExperiment,numeric'
values(object) <- value
```

Arguments

| | |
|--------|-----------------------------------|
| object | SummarizedExperiment |
| value | ratio matrix (features x samples) |

Value

value matrix (get) or updated object (set)

Examples

```
file <- download_data('billing16.proteingroups.txt')
object <- read_proteingroups(file, plot=FALSE)
values(object)[1:3, 1:3]
values(object) <- 0
values(object)[1:3, 1:3]
```

venn_detects *Venn detects*

Description

Venn diagram full/systematic/random detects

Usage

```
venn_detects(object, subgroup)
```

Arguments

| | |
|----------|----------------------|
| object | SummarizedExperiment |
| subgroup | subgroup symbol |

Value

NULL

Examples

```
file <- download_data('fukuda20.proteingroups.txt')
object <- read_proteingroups(file, impute=FALSE, plot = FALSE)
venn_detects(object, subgroup)
```

weights *Get/Set weights*

Description

Get/Set weight matrix

Usage

```
weights(object, ...)

## S4 method for signature 'SummarizedExperiment'
weights(object)

weights(object) <- value

## S4 replacement method for signature 'SummarizedExperiment,matrix'
weights(object) <- value

## S4 replacement method for signature 'SummarizedExperiment,numeric'
```

```
weights(object) <- value

## S4 replacement method for signature 'SummarizedExperiment,`NULL`'
weights(object) <- value
```

Arguments

| | |
|--------|-----------------------------------|
| object | SummarizedExperiment |
| ... | additional params |
| value | ratio matrix (features x samples) |

Value

weight matrix (get) or updated object (set)

Examples

```
file <- download_data('billing19.proteingroups.txt')
object <- read_proteingroups(file, plot=FALSE)
weights(object)[1:3, 1:2]
weights(object) <- 1; weights(object)[1:3, 1:2]
```

| | |
|------------|--|
| zero_to_na | <i>Change nondetect representation</i> |
|------------|--|

Description

Change nondetect representation

Usage

```
zero_to_na(x, verbose = FALSE)

nan_to_na(x, verbose = FALSE)

na_to_zero(x, verbose = FALSE)

inf_to_na(x, verbose = FALSE)

minusinf_to_na(x, verbose = FALSE)
```

Arguments

| | |
|---------|------------|
| x | matrix |
| verbose | logical(1) |

Value

Updated matrix

Examples

```
require(magrittr)
matrix(c(0, 7), nrow=1)
matrix(c(0, 7), nrow=1) %>% zero_to_na(verbose=TRUE)

matrix(c(NA, 7), nrow=1)
matrix(c(NA, 7), nrow=1) %>% na_to_zero(verbose=TRUE)

matrix(c(NaN, 7), nrow=1)
matrix(c(NaN, 7), nrow=1) %>% nan_to_na(verbose=TRUE)

matrix(c(Inf, 7), nrow=1)
matrix(c(Inf, 7), nrow=1) %>% inf_to_na(verbose=TRUE)

matrix(c(-Inf, 7), nrow=1)
matrix(c(-Inf, 7), nrow=1) %>% minusinf_to_na(verbose=TRUE)
```

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