

Package ‘autonomics’

May 25, 2023

Type Package

Title Generifying and intuitifying cross-platform omics analysis

Version 1.9.0

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, 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, tidyr, 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 devel

git_last_commit b7118ef

git_last_commit_date 2023-04-25

Date/Publication 2023-05-25

Author Aditya Bhagwat [aut, cre],
 Shahina Hayat [aut],
 Anna Halama [ctb],
 Richard Cotton [ctb],
 Laure Cougnaud [ctb],
 Rudolf Engelke [ctb],
 Hinrich Goehlmann [sad],
 Karsten Suhre [sad],
 Johannes Graumann [aut, sad, rth]

Maintainer Aditya Bhagwat <aditya.bhagwat@uni-marburg.de>

R topics documented:

.read_maxquant	4
.read_metabolon	7
.read_rectangles	8
.read_rnaseq_bams	11
.read_somascan	14
add_smiles	16
analysis	16
analyze	17
assert_is_valid_sumexp	18
AUTONOMICS_DATASETS	19
biplot	20
center	21
contrastdefs	22
contrast_subgroup_cols	22
counts	23
counts2cpm	24
counts2tpm	25
cpm	25
create_design	26
create_sfile	27
default_sfile	28
default_subgroupvar	28
download_data	29
download_gtf	30
dt2mat	31
explore_imputations	32
explore_transformations	32
extract_features	33

extract_rectangle	34
fdata	36
filter_exprs_replicated_in_some_subgroup	37
filter_features	38
filter_medoid	39
filter_replicated	39
filter_samples	40
fit_limma	41
flevels	43
fnames	43
formula2str	44
fvalues	45
fvars	45
guess_maxquant_quantity	46
guess_sep	47
impute_systematic_nondetects	48
invert	49
is_imputed	50
is_sig	51
limma	52
log2counts	53
log2countsratios	54
log2cpm	55
log2cpmratios	56
log2tpm	57
log2tpmratios	58
log2transform	59
make_volcano_dt	60
matrix2sumexp	60
MAXQUANT_PATTERNS_PEP COUNTS	61
MAXQUANT_PATTERNS_QUANTITY	62
merge_sdata	62
merge_sfile	63
message_df	65
nfactors	65
normimpute	66
occupancies	67
pca	68
plot_boxplots	69
plot_contrastogram	71
plot_corrections	72
plot_covariates	73
plot_data	74
plot_densities	75
plot_detects	77
plot_features	78
plot_venn	79
plot_violins	80

plot_volcano	81
preprocess_rnaseq_counts	82
proteingroups	83
read_affymetrix	84
rm_singleton_samples	85
scaledlibsizes	86
sdata	86
slevels	87
snames	88
split_by_svar	89
standardize_maxquant_snames	89
subgroup_array	91
subtract_baseline	91
sumexp2mae	93
sumexp_to_wide_dt	94
summarize_fit	95
svalues	96
svars	97
TESTS	98
tpm	98
values	99
venn_detects	100
weights	100
zero_to_na	101

Index**103**

<i>.read_maxquant</i>	<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 cor-

	rected", "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	<i>Read omics data from rectangular file</i>
------------------	--

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)

```

<i>.read_rnaseq_bams</i>	<i>Read rnaseq</i>
--------------------------	--------------------

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

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

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

Analyze

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 12.

Examples

AUTONOMICS_DATASETS

biplot	<i>Biplot</i>
--------	---------------

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

object	SummarizedExperiment
x	pca1, etc.
y	pca2, etc.
color	svar mapped to color (symbol)
group	svar mapped to group
label	svar mapped to label (symbol)
feature_label	fvar mapped to (loadings) label
...	additional svars mapped to aesthetics
fixed	fixed plot aesthetics
nloadings	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	<i>Convert between counts and cpm</i>
------------	---------------------------------------

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	Create sfile
--------------	--------------

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
	• Billing 2016: stemcell comparison: E, EM, BM – 'billing16.bam.zip' – 'billing16.rnacounts.txt' – 'billing16.somascan.adat' – 'billing16.proteingroups.txt' • Atkin 2018: hypoglycemia: t0, t1, t2, t3 – 'atkin18.somascan.adat' – 'atkin18.metbolon.xlsx' • Halama 2018: glutaminase inhibition: 4 conc, 4 timepoints – 'halama18.metabolon.xlsx' • Billing 2019: stemcell differentiation: E00, E01, E02, E05, EM15, EM30, M00 – 'billing19.rnacounts.txt' – 'billing19.proteingroups.txt' – 'billing19.phosphosites.txt' • Fukuda 2020: zebrafish development: X30dpt, Adult – '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 PXD016235
  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	<i>Explore imputations</i>
---------------------	----------------------------

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	<i>Explore transformations</i>
-------------------------	--------------------------------

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	<i>Extract rectangle from omics file, data.table, or matrix</i>
-------------------	---

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

<code>x</code>	omics datafile or datatable
<code>...</code>	allow for S3 method dispatch
<code>rows</code>	numeric vector
<code>cols</code>	numeric vector
<code>verbose</code>	logical
<code>transpose</code>	logical
<code>drop</code>	logical
<code>sheet</code>	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 • c("t1-t0", "t2-t1", "t3-t2") • 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) • 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))
block	block svar (or NULL)
weightvar	NULL or name of weight matrix in assays(object)
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	<i>formula to string</i>
-------------	--------------------------

Description

formula to string

Usage

```
formula2str(formula)
```

Arguments

formula formula

Value

string

Examples

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

fvalues	<i>Get fvalues</i>
---------	--------------------

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	<i>Get/Set fvars</i>
-------	----------------------

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

<code>x</code>	character vector or SummarizedExperiment
<code>...</code>	used for proper S3 method dispatch
<code>separators</code>	character vector: possible separators to look for
<code>verbose</code>	TRUE or FALSE
<code>var</code>	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(  
  object,
```

```

    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

Get/set is_imputed

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 autonomics::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`*Get/Set log2cpm*

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

<code>object</code>	SummarizedExperiment
<code>value</code>	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`*Get/Set log2tpm*

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

<code>object</code>	SummarizedExperiment
<code>value</code>	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	Create volcano datatable
-----------------	--------------------------

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	Convert matrix into SummarizedExperiment
---------------	--

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_PEPCOUNTS

maxquant peptide count patterns

Description

maxquant peptide count patterns

Usage

MAXQUANT_PATTERNS_PEPCOUNTS

Format

An object of class character of length 3.

Examples

MAXQUANT_PATTERNS_PEPCOUNTS

MAXQUANT_PATTERNS_QUANTITY
<i>maxquant quantity patterns</i>

Description

maxquant quantity patterns

Usage

MAXQUANT_PATTERNS_QUANTITY

Format

An object of class character of length 7.

Examples

MAXQUANT_PATTERNS_QUANTITY

merge_sdata	<i>Merge sample/feature data</i>
-------------	----------------------------------

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 mergevvar
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	which mean to impute around

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	<i>Plot sample/feature boxplots</i>
---------------	-------------------------------------

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	<i>Plot contrastogram</i>
--------------------	---------------------------

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	<i>Biplot batch corrections</i>
------------------	---------------------------------

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	<i>Plot data</i>
-----------	------------------

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	<i>Plot sample/feature densities</i>
----------------	--------------------------------------

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 compatibility
object	SummarizedExperiment
subgroup	subgroup var (sym)
fill	fill var (sym)
na_imputes	whether to NA imputes prior to plotting (TRUE/FALSE)

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	<i>Plot features</i>
---------------	----------------------

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	<i>Plot volcano</i>
--------------	---------------------

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(celfiles = 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	<i>Get slevels</i>
---------	--------------------

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	<i>Get/Set snames</i>
--------	-----------------------

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	<i>Convert SummarizedExperiment into data.table</i>
-------------------	---

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	<i>Summarize fit</i>
---------------	----------------------

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	<i>Get/Set svalues</i>
---------	------------------------

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	<i>Venn detects</i>
--------------	---------------------

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	<i>Get/Set weights</i>
---------	------------------------

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)
```

Index

* datasets

AUTONOMICS_DATASETS, [19](#)
MAXQUANT_PATTERNS_PEP_COUNTS, [61](#)
MAXQUANT_PATTERNS_QUANTITY, [62](#)
TESTS, [98](#)
.read_maxquant, [4](#)
.read_metabolon, [7](#)
.read_rectangles, [8](#)
.read_rnaseq_bams, [11](#)
.read_rnaseq_counts
 (.read_rnaseq_bams), [11](#)
.read_somascan, [14](#)
add_smiles, [16](#)
analysis, [16](#)
analysis, SummarizedExperiment-method
 (analysis), [16](#)
analysis<- (analysis), [16](#)
analysis<-, SummarizedExperiment, list-method
 (analysis), [16](#)
analyze, [17](#)
assert_is_valid_sumexp, [18](#)
AUTONOMICS_DATASETS, [19](#)

biplot, [20](#)
biplot_corrections (plot_corrections),
 [72](#)
biplot_covariates (plot_covariates), [73](#)

center, [21](#)
contrast_subgroup_cols, [22](#)
contrast_subgroup_rows
 (contrast_subgroup_cols), [22](#)
contrastdefs, [22](#)
contrastdefs, SummarizedExperiment-method
 (contrastdefs), [22](#)
contrastdefs<- (contrastdefs), [22](#)
contrastdefs<-, SummarizedExperiment, list-method
 (contrastdefs), [22](#)
counts, [23](#)
counts, SummarizedExperiment-method
 (counts), [23](#)
counts2cpm, [24](#)
counts2tpm, [25](#)
counts<- (counts), [23](#)
counts<-, SummarizedExperiment, matrix-method
 (counts), [23](#)
counts<-, SummarizedExperiment, NULL-method
 (counts), [23](#)
counts<-, SummarizedExperiment, numeric-method
 (counts), [23](#)
cpm, [25](#)
cpm, SummarizedExperiment-method (cpm),
 [25](#)
cpm2counts (counts2cpm), [24](#)
cpm<- (cpm), [25](#)
cpm<-, SummarizedExperiment, matrix-method
 (cpm), [25](#)
cpm<-, SummarizedExperiment, numeric-method
 (cpm), [25](#)
create_design, [26](#)
create_sfile, [27](#)

default_formula (default_subgroupvar),
 [28](#)
default_sfile, [28](#)
default_subgroupvar, [28](#)
download_data, [29](#)
download_gtf, [30](#)
dt2mat, [31](#)

exp2 (log2transform), [59](#)
explore_imputations, [32](#)
explore_transformations, [32](#)
extract_features, [33](#)
extract_rectangle, [34](#)

fdata, [36](#)
fdata, SummarizedExperiment-method
 (fdata), [36](#)

fdata<- (fdata), 36
 fdata<- , SummarizedExperiment, data.frame-method
 (fdata), 36
 filter_exprs_replicated_in_some_subgroup,
 37
 filter_features, 38
 filter_medoid, 39
 filter_replicated, 39
 filter_samples, 40
 fit_limma, 41
 fit_lm (fit_limma), 41
 fit_lme (fit_limma), 41
 fit_lmer (fit_limma), 41
 fit_wilcoxon (fit_limma), 41
 flevels, 43
 fnames, 43
 fnames, SummarizedExperiment-method
 (fnames), 43
 fnames<- (fnames), 43
 fnames<- , SummarizedExperiment, character-method
 (fnames), 43
 formula2str, 44
 fvalues, 45
 fvars, 45
 fvars, SummarizedExperiment-method
 (fvars), 45
 fvars<- (fvars), 45
 fvars<- , SummarizedExperiment, character-method
 (fvars), 45

 guess_maxquant_quantity, 46
 guess_sep, 47

 halfnormimpute (normimpute), 66

 impute_systematic_nondetects, 48
 inf_to_na (zero_to_na), 101
 invert, 49
 invnorm (log2transform), 59
 is_imputed, 50
 is_imputed, SummarizedExperiment-method
 (is_imputed), 50
 is_imputed<- (is_imputed), 50
 is_imputed<- , SummarizedExperiment, matrix-method
 (is_imputed), 50
 is_imputed<- , SummarizedExperiment, NULL-method
 (is_imputed), 50
 is_sig, 51
 lda (pca), 68

 limma, 52
 limma, SummarizedExperiment-method
 (limma), 52
 limma<- (limma), 52
 limma<- , SummarizedExperiment, array-method
 (limma), 52
 limma<- , SummarizedExperiment, NULL-method
 (limma), 52
 log2counts, 53
 log2counts, SummarizedExperiment-method
 (log2counts), 53
 log2counts<- (log2counts), 53
 log2counts<- , SummarizedExperiment, matrix-method
 (log2counts), 53
 log2counts<- , SummarizedExperiment, numeric-method
 (log2counts), 53
 log2countsratios, 54
 log2countsratios, SummarizedExperiment-method
 (log2countsratios), 54
 log2countsratios<- (log2countsratios),
 54
 log2countsratios<- , SummarizedExperiment, matrix-method
 (log2countsratios), 54
 log2countsratios<- , SummarizedExperiment, numeric-method
 (log2countsratios), 54
 log2cpm, 55
 log2cpm, SummarizedExperiment-method
 (log2cpm), 55
 log2cpm<- (log2cpm), 55
 log2cpm<- , SummarizedExperiment, matrix-method
 (log2cpm), 55
 log2cpm<- , SummarizedExperiment, numeric-method
 (log2cpm), 55
 log2cpmratios, 56
 log2cpmratios, SummarizedExperiment-method
 (log2cpmratios), 56
 log2cpmratios<- (log2cpmratios), 56
 log2cpmratios<- , SummarizedExperiment, matrix-method
 (log2cpmratios), 56
 log2cpmratios<- , SummarizedExperiment, numeric-method
 (log2cpmratios), 56
 log2tpm, 57
 log2tpm, SummarizedExperiment-method
 (log2tpm), 57
 log2tpm<- (log2tpm), 57
 log2tpm<- , SummarizedExperiment, matrix-method
 (log2tpm), 57
 log2tpm<- , SummarizedExperiment, numeric-method

- (log2tpm), 57
- log2tpmratios, 58
- log2tpmratios, SummarizedExperiment-method
(log2tpmratios), 58
- log2tpmratios<- (log2tpmratios), 58
- log2tpmratios<- , SummarizedExperiment, matrix-method
(log2tpmratios), 58
- log2tpmratios<- , SummarizedExperiment, numeric-method
(log2tpmratios), 58
- log2transform, 59
- make_volcano_dt, 60
- mat2dt (dt2mat), 31
- matrix2sumexp, 60
- MAXQUANT_PATTERNS_PEP COUNTS, 61
- MAXQUANT_PATTERNS_QUANTITY, 62
- merge_fdata (merge_sdata), 62
- merge_ffile (merge_sfile), 63
- merge_sdata, 62
- merge_sfile, 63
- message_df, 65
- minusinf_to_na (zero_to_na), 101
- na_to_zero (zero_to_na), 101
- nan_to_na (zero_to_na), 101
- nfactors, 65
- normimpute, 66
- occupancies, 67
- occupancies, SummarizedExperiment-method
(occupancies), 67
- occupancies<- (occupancies), 67
- occupancies<- , SummarizedExperiment, matrix-method
(occupancies), 67
- occupancies<- , SummarizedExperiment, numeric-method
(occupancies), 67
- pca, 68
- plot_biplot (biplot), 20
- plot_boxplots, 69
- plot_contrastogram, 71
- plot_corrections, 72
- plot_covariates, 73
- plot_data, 74
- plot_densities, 75
- plot_detections (plot_detects), 77
- plot_detects, 77
- plot_feature_boxplots (plot_boxplots), 69
- plot_feature_densities
(plot_densities), 75
- plot_feature_profiles (plot_features), 78
- plot_feature_violins (plot_violins), 80
- plot_features, 78
- plot_quantifications (plot_detects), 77
- plot_sample_boxplots, 76, 81
- plot_sample_boxplots (plot_boxplots), 69
- plot_sample_densities, 70, 81
- plot_sample_densities (plot_densities), 75
- plot_sample_violins, 70, 76
- plot_sample_violins (plot_violins), 80
- plot_subgroup_boxplots (plot_boxplots), 69
- plot_subgroup_violins (plot_violins), 80
- plot_summarized_detections
(plot_detects), 77
- plot_venn, 79
- plot_violins, 80
- plot_volcano, 81
- plotmat, 71
- pls (pca), 68
- preprocess_rnaseq_counts, 82
- proteingroups, 83
- proteingroups, SummarizedExperiment-method
(proteingroups), 83
- proteingroups<- (proteingroups), 83
- proteingroups<- , SummarizedExperiment, matrix-method
(proteingroups), 83
- proteingroups<- , SummarizedExperiment, numeric-method
(proteingroups), 83
- quantnorm (log2transform), 59
- read_affymetrix, 84
- read_metabolon (.read_metabolon), 7
- read_phosphosites (.read_maxquant), 4
- read_proteingroups (.read_maxquant), 4
- read_rectangles (.read_rectangles), 8
- read_rnaseq_bams (.read_rnaseq_bams), 11
- read_rnaseq_counts (.read_rnaseq_bams), 11
- read_somascan (.read_somascan), 14
- rm_singleton_samples, 85
- sampleid_values (svalues), 96
- scaledlibsizes, 86

sdata, 86
 sdata, MultiAssayExperiment-method
 (sdata), 86
 sdata, SummarizedExperiment-method
 (sdata), 86
 sdata<- (sdata), 86
 sdata<-, MultiAssayExperiment, data.frame-method
 (sdata), 86
 sdata<-, MultiAssayExperiment, DataFrame-method
 (sdata), 86
 sdata<-, SummarizedExperiment, data.frame-method
 (sdata), 86
 sdata<-, SummarizedExperiment, DataFrame-method
 (sdata), 86
 slevels, 87
 sma (pca), 68
 snames, 88
 snames, SummarizedExperiment-method
 (snames), 88
 snames<- (snames), 88
 snames<-, SummarizedExperiment, character-method
 (snames), 88
 split_by_svar, 89
 split_extract (nfactors), 65
 standardize_maxquant_snames, 89
 subgroup_array, 91
 subgroup_levels (slevels), 87
 subgroup_matrix (subgroup_array), 91
 subgroup_values (svalues), 96
 subtract_baseline, 91
 subtract_differences
 (subtract_baseline), 91
 subtract_pairs (subtract_baseline), 91
 sumexp2mae, 93
 sumexp_to_long_dt (sumexp_to_wide_dt),
 94
 sumexp_to_subrep_dt
 (sumexp_to_wide_dt), 94
 sumexp_to_wide_dt, 94
 summarize_fit, 95
 svalues, 96
 svalues<- (svalues), 96
 svalues<-, SummarizedExperiment, character-method
 (svalues), 96
 svars, 97
 svars, MultiAssayExperiment-method
 (svars), 97
 svars, SummarizedExperiment-method
 (svars), 97
 svars<- (svars), 97
 svars<-, MultiAssayExperiment, character-method
 (svars), 97
 svars<-, SummarizedExperiment, character-method
 (svars), 97
 TESTS, 98
 tpm, 98
 tpm, SummarizedExperiment-method (tpm),
 98
 tpm<- (tpm), 98
 tpm<-, SummarizedExperiment, matrix-method
 (tpm), 98
 tpm<-, SummarizedExperiment, numeric-method
 (tpm), 98
 translate (normimpute), 66
 values, 99
 values, SummarizedExperiment-method
 (values), 99
 values<- (values), 99
 values<-, SummarizedExperiment, matrix-method
 (values), 99
 values<-, SummarizedExperiment, numeric-method
 (values), 99
 venn_detects, 100
 weights, 100
 weights, SummarizedExperiment-method
 (weights), 100
 weights<- (weights), 100
 weights<-, SummarizedExperiment, matrix-method
 (weights), 100
 weights<-, SummarizedExperiment, NULL-method
 (weights), 100
 weights<-, SummarizedExperiment, numeric-method
 (weights), 100
 zero_to_na, 101
 zeroimpute (normimpute), 66
 zscore (log2transform), 59