

# Package ‘autonomics’

April 10, 2023

**Type** Package

**Title** Generify and intuifying cross-platform omics analysis

**Version** 1.6.0

**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>

**RoxxygenNote** 7.1.1

**Depends** R (>= 4.0)

**Imports** abind, assertive, BiocFileCache, BiocGenerics, colorspace,  
data.table, edgeR, ggplot2, ggrepel, graphics, grDevices, grid,  
gridExtra, limma, magrittr, matrixStats, methods,  
MultiAssayExperiment, parallel, pcaMethods, rappdirs, rlang,  
R.utils, readxl, S4Vectors, scales, stats, stringi,  
SummarizedExperiment, tidyverse, tools, utils

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

**git\_url** <https://git.bioconductor.org/packages/autonomics>

**git\_branch** RELEASE\_3\_16  
**git\_last\_commit** 6768188  
**git\_last\_commit\_date** 2022-11-01

**Date/Publication** 2023-04-10

**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 . . . . .	6
.read_rectangles . . . . .	8
.read_rnaseq_bams . . . . .	11
.read_somascan . . . . .	14
add_smiles . . . . .	15
analysis . . . . .	16
analyze . . . . .	17
assert_is_valid_sumexp . . . . .	18
AUTONOMICS_DATASETS . . . . .	19
biplot . . . . .	19
center . . . . .	20
contrastdefs . . . . .	21
contrast_subgroup_cols . . . . .	22
counts . . . . .	23
counts2cpm . . . . .	24
counts2tpm . . . . .	24
cpm . . . . .	25
create_design . . . . .	26
create_sfile . . . . .	27
default_sfile . . . . .	27
default_subgroupvar . . . . .	28
download_data . . . . .	29
download_gtf . . . . .	30
dt2mat . . . . .	31
explore_imputations . . . . .	31
explore_transformations . . . . .	32
extract_features . . . . .	33
extract_rectangle . . . . .	34

fdata . . . . .	36
filter_exprs_replicated_in_some_subgroup . . . . .	37
filter_features . . . . .	38
filter_medoid . . . . .	38
filter_replicated . . . . .	39
filter_samples . . . . .	40
fit_limma . . . . .	40
flevels . . . . .	42
fnames . . . . .	43
formula2str . . . . .	44
fvalues . . . . .	44
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_PEPCOUNTS . . . . .	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 . . . . .	76
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_PEPCOUNTS[1],
    subgroupvar = NULL,
    formula = NULL,
    block = NULL,
    contrastdefs = NULL,
    pca = FALSE,
    fit = NULL,
    verbose = TRUE,
    plot = TRUE
)
read_phosphosites(
  file,
  proteininfile = paste0(dirname(file), "/proteinGroups.txt"),
  quantity = guess_maxquant_quantity(file),
  sfile = NULL,
  sfileby = NULL,
  select_subgroups = NULL,
  contaminants = FALSE,
  reverse = FALSE,
  min_localization_prob = 0.75,
  fastafile = NULL,
  invert_subgroups = character(0),
  pca = FALSE,
  fit = NULL,
  subgroupvar = NULL,
  formula = NULL,
  block = NULL,
  contrastdefs = NULL,
  verbose = TRUE,
  plot = TRUE
)
```

## Arguments

file	proteingroups/phosphosites file
quantity	string: "Ratio normalized", "Ratio", "LFQ intensity", "Reporter intensity corrected", "Reporter intensity", "Intensity labeled", "Intensity"

```

sfile      sample file
sfileby    sample file mergeby column
subgroupvar subgroup svar
select_subgroups
            subgroups to be selected (character vector)
invert_subgroups
            subgroups to be inverted (character vector)
pepcountpattern
            value in MAXQUANT_PATTERNS_PEPCOUNTS
verbose    whether to message
contaminants whether to return contaminants
reverse    whether to return reverse peptides
fastafile  NULL or fastaf file (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*      *Read metabolon*

### **Description**

Read metabolon

### Usage

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

### Arguments

file	metabolon xlsx filepath
sheet	xls sheet number or name
fid_var	feature_id fvar
sid_var	sampleid svar
sfile	sample file
sfileby	sample file mergeby column
by	metabolon file mergeby column
subgroupvar	subgroup svar
fname_var	featurename fvar
impute	whether to impute

```

add_kegg_pathways           whether to add kegg pathways
add_smiles                 whether to add smiles
pca                        whether to pca
fit                         fit model: NULL, 'limma', 'lm', 'lme', 'lmer', 'wilcoxon'
formula                     designmat formula
block                       block svar
contrastdefs               contrastdef vector/matrix/list
verbose                     whether to msg
plot                        whether to plot

```

**Value**

SummarizedExperiment

**Examples**

```

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

```

**.read\_rectangles**      *Read omics data from rectangular file*

**Description**

Read omics data from rectangular file

**Usage**

```

.read_rectangles(
  file,
  sheet = 1,
  fid_rows,
  fid_cols,
  sid_rows,
  sid_cols,
  expr_rows,
  expr_cols,
  fvar_rows = NULL,
  fvar_cols = NULL,
  svar_rows = NULL,
  svar_cols = NULL,
  fdata_rows = NULL,
  fdata_cols = NULL,
  sdata_rows = NULL,

```

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

## Arguments

file	string: name of text (txt, csv, tsv, adat) or excel (xls, xlsx) file
sheet	integer/string: only relevant for excel files
fid_rows	numeric vector: featureid rows
fid_cols	numeric vector: featureid cols
sid_rows	numeric vector: sampleid rows
sid_cols	numeric vector: sampleid cols
expr_rows	numeric vector: expr rows
expr_cols	numeric vector: expr cols
fvar_rows	numeric vector: fvar rows
fvar_cols	numeric vector: fvar cols
svar_rows	numeric vector: svar rows
svar_cols	numeric vector: svar cols
fdata_rows	numeric vector: fdata rows
fdata_cols	numeric vector: fdata cols

sdata_rows	numeric vector: sdata rows
sdata_cols	numeric vector: sdata cols
transpose	TRUE or FALSE (default)
verbose	TRUE (default) or FALSE
sfile	sample file
sfileby	sample file mergeby column
subgroupvar	subgroupvar in sfile

**Value**

SummarizedExperiment

**Examples**

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

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

# SOMASCAN
  file <- download_data('billing16.somascan.adat')
  read_rectangles(file,fid_rows = 21,      fid_cols = 19:1146,
                  sid_rows = 30:40,    sid_cols = 4,
                  expr_rows = 30:40,   expr_cols = 19:1146,
                  fvar_rows = 21:28,   fvar_cols = 18,
                  svar_rows = 29,       svar_cols = 1:17,
                  fdata_rows = 21:28,  fdata_cols = 19:1146,
                  sdata_rows = 30:40,  sdata_cols = 1:17,
                  transpose = TRUE)

# METABOLON
  file <- download_data('halama18.metabolon.xlsx')
  read_rectangles(file, sheet = 2,
                  fid_rows = 11:401,   fid_cols = 5,
                  sid_rows = 3,         sid_cols = 15:86,
                  expr_rows = 11:401,   expr_cols = 15:86,
                  fvar_rows = 10,        fvar_cols = 1:14,
                  svar_rows = 1:10,       svar_cols = 14,
                  fdata_rows = 11:401,  fdata_cols = 1:14,
                  sdata_rows = 1:10,     sdata_cols = 15:86,
                  transpose = FALSE)
```

---

.read\_rnaseq\_bams      *Read rnaseq*

---

## Description

Read/analyze rnaseq counts / bamfiles

## Usage

```
.read_rnaseq_bams(  
  dir,  
  paired,  
  genome,  
  nthreads = detectCores(),  
  sfile = NULL,  
  sfileby = NULL,  
  subgroupvar = NULL,  
  ffile = NULL,  
  ffileby = NULL,  
  fnamevar = NULL,  
  verbose = TRUE  
)  
  
.read_rnaseq_counts(  
  file,  
  fid_col = 1,  
  sfile = NULL,  
  sfileby = NULL,  
  ffile = NULL,  
  ffileby = NULL,  
  subgroupvar = NULL,  
  verbose = TRUE  
)  
  
read_rnaseq_bams(  
  dir,  
  paired,  
  genome,  
  nthreads = detectCores(),  
  sfile = NULL,  
  sfileby = NULL,  
  subgroupvar = NULL,  
  block = NULL,  
  ffile = NULL,  
  ffileby = NULL,  
  fnamevar = NULL,  
  formula = NULL,
```

```

min_count = 10,
pseudocount = 0.5,
genesize = NULL,
cpm = TRUE,
tmm = cpm,
log2 = TRUE,
pca = FALSE,
fit = NULL,
voom = !is.null(fit),
contrastdefs = NULL,
verbose = TRUE,
plot = TRUE
)

read_rnaseq_counts(
  file,
  fid_col = 1,
  sfile = NULL,
  sfileby = NULL,
  subgroupvar = NULL,
  block = NULL,
  ffile = NULL,
  ffileby = NULL,
  fnamevar = NULL,
  formula = NULL,
  min_count = 10,
  pseudocount = 0.5,
  genesize = NULL,
  cpm = TRUE,
  tmm = cpm,
  log2 = TRUE,
  pca = FALSE,
  fit = NULL,
  voom = !is.null(fit),
  contrastdefs = NULL,
  verbose = TRUE,
  plot = TRUE
)

```

## Arguments

dir	<code>read_rnaseq_bams</code> : bam/samfile dir
paired	<code>read_rnaseq_bams</code> : whether paired end reads
genome	<code>read_rnaseq_bams</code> : mm10/"hg38"/etc. or GTF file
nthreads	<code>read_rnaseq_bams</code> : nthreads used by <code>Rsubread::featureCounts()</code>
sfile	sample file
sfileby	sample file mergeby column

subgroupvar	subgroup svar
ffile	feature file
ffileby	feature file mergeby column
fnamevar	featurename fvar
verbose	whether to message
file	read_rnaseq_counts: count file
fid_col	featureid fvar
block	block svar
formula	designmat formula
min_count	min feature count required in some samples
pseudocount	added pseudocount to prevent -Inf log2 values
genesize	genesize fvar for tpm
cpm	whether to compute cpm
tmm	whether to tmm-scale library sizes
log2	whether to log2 transform
pca	whether to pca
fit	fit model: NULL, 'limma', 'lme', 'lmer', 'wilcoxon'
voom	whether to compute voom precision weights
contrastdefs	contrastdef vector/matrix/list
plot	whether to plot

**Value**

SummarizedExperiment

**Author(s)**

Aditya Bhagwat, Shahina Hayat

**Examples**

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

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

---

.read_somascan	<i>Read somascan</i>
----------------	----------------------

---

## Description

Read data from somascan adat file

## Usage

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

read_somascan(
  file,
  fidvar = "SeqId",
  sidvar = "SampleId",
  sfile = NULL,
  sfileby = NULL,
  by = NULL,
  subgroupvar = "SampleGroup",
  fname_var = "EntrezGeneSymbol",
  sample_type = "Sample",
  feature_type = "Protein",
  sample_quality = c("FLAG", "PASS"),
  feature_quality = c("FLAG", "PASS"),
  rm_na_svars = FALSE,
  rm_single_value_svars = FALSE,
  pca = FALSE,
  fit = NULL,
  formula = NULL,
  block = NULL,
  contrastdefs = NULL,
  verbose = TRUE,
  plot = TRUE
)
```

## Arguments

file	*.adat file path (string)
fidvar	featureid fvar (string)

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

**Value**

Summarizedexperiment

**Examples**

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

---

add\_smiles

*Add smiles*

---

**Description**

Add smiles

**Usage**

add\_smiles(object)

**Arguments**

object	character/factor vector with pubchem ids
--------	--

**Value**

character/factor vector
-------------------------

**References**

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

**Examples**

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

analysis

*Get/set analysis***Description**

Get/set analysis

**Usage**

```
analysis(object)

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

analysis(object) <- value

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

**Arguments**

object	SummarizedExperiment
value	list

**Value**

analysis details (get) or updated object (set)

**Examples**

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

---

**analyze***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                          *Biplot*

---

**Description**

Biplot

**Usage**

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

**Arguments**

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 svards 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

*Center samples*

**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

*Get/set contrastdefs***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**

*Row/Col contrasts*

**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	<i>Get/Set counts</i>
--------	-----------------------

---

## 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('billig19.rnacounts.txt')
object <- read_rnased_counts(file, plot=FALSE)
counts(object) <- values(object)
counts(object)[1:3, 1:3]
```

counts2cpm

*Convert between counts and cpm***Description**

Convert between counts and cpm

**Usage**

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

cpm2counts(x, libsize)
```

**Arguments**

x	count/cpm matrix
libsize	(scaled) libsize vector

**Value**

cpm/tpm/count matrix

**Examples**

```
file <- download_data('billing19.rnacounts.txt')
object <- read_rnased_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

*counts to tpm***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_rnased_counts(file, cpm=FALSE, log2=FALSE, plot=FALSE)
counts2tpm(counts(object), genesize=1)[1:3, 1:3]
```

---

cpm

*Get/Set cpm*

---

**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_rnased_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**

<code>object</code>	SummarizedExperiment
<code>subgroupvar</code>	subgroup svar
<code>formula</code>	formula with svars
<code>verbose</code>	whether to message

**Value**

design matrix

**Examples**

```
file <- download_data('billing19.rnacounts.txt')
object <- read_rnasedq_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

*Default sfile*

---

### 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**     *Create default formula*

**Description**

Create default formula

**Usage**

```
default_subgroupvar(object)

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

**Arguments**

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

**Value**

formula

**Examples**

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

---

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

---

## Description

Download autonomics example data

## Usage

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

## Arguments

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

---

**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**

*Explore transformations*

**Description**

Explore transformations

**Usage**

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

**Arguments**

object	SummarizedExperiment
subgroup	subgroup (sym)
transformations	vector
method	'pca', 'pls', 'sma', or 'lda'

```
xdim      number (default 1)
ydim      number (default 2)
...       passed to plot_data
```

**Value**

grid object

**Examples**

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

---

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

---

**Description**

Extract features

**Usage**

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

**Arguments**

object	SummarizedExperiment
extractor	logical/numeric vector

**Value**

SummarizedExperiment

**Examples**

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

---

extract_rectangle	<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

x	omics datafile or datatable
...	allow for S3 method dispatch

rows	numeric vector
cols	numeric vector
verbose	logical
transpose	logical
drop	logical
sheet	numeric or string

**Value**

matrix

**Examples**

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

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

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

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

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

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

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

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

```

  extract(,1:3)

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

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

```

---

**fdata***Get/Set fdata***Description**

Get/Set feature data

**Usage**

```

fdata(object)

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

fdata(object) <- value

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

```

**Arguments**

object	SummarizedExperiment, eSet, or EList
value	data.frame

**Value**

feature dataframe (get) or updated object (set)

**Examples**

```

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

```

---

```
filter_exprs_replicated_in_some_subgroup
```

*Filter features with replicated expression in some subgroup*

---

## Description

Filter features with replicated expression in some subgroup

## Usage

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

## Arguments

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

## Value

Filtered SummarizedExperiment

## Examples

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

**filter\_features**      *Filter features on condition*

### 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**      *Filter medoid sample*

### 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      *Filter for replicated features*

---

**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**      *Filter samples on condition*

### 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**

<b>object</b>	SummarizedExperiment
<b>subgroupvar</b>	subgroup variable
<b>formula</b>	modeling formula
<b>contrastdefs</b>	contrastdef vector / matrix / list <ul style="list-style-type: none"><li>• c("t1-t0", "t2-t1", "t3-t2")</li><li>• 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)</li><li>• 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))</li></ul>
<b>block</b>	block svar (or NULL)
<b>weightvar</b>	NULL or name of weight matrix in assays(object)
<b>verbose</b>	whether to msg
<b>plot</b>	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'))
```

**Description**

Get fvar levels

**Usage**

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

**Arguments**

object	SummarizedExperiment
fvar	feature variable

**Value**

fvar values

**Examples**

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

---

fnames

*Get/Set fnames*

---

**Description**

Get/Set feature names

**Usage**

```
fnames(object)

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

fnames(object) <- value

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

**Arguments**

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

**Value**

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

**Examples**

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

formula2str

*formula to string***Description**

formula to string

**Usage**

formula2str(formula)

**Arguments**

formula formula

**Value**

string

**Examples**

formula2str(~0+subgroup)

fvalues

*Get fvalues***Description**

Get fvar values

**Usage**

fvalues(object, fvar)

**Arguments**

object	SummarizedExperiment
fvar	feature variable

**Value**

fvar values

**Examples**

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

---

fvars

*Get/Set fvars*

---

**Description**

Get/Set feature variables

**Usage**

```
fvars(object)

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

fvars(object) <- value

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

**Arguments**

object	SummarizedExperiment
value	character vector with feature variables

**Value**

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

**Examples**

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

**guess\_maxquant\_quantity***Guess maxquant quantity from snames***Description**

character vector, dataframe, or SummarizedExperiment.

**Usage**

```
guess_maxquant_quantity(x, ...)

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

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

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

**Arguments**

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

**Value**

string: value from names(MAXQUANT\_PATTERNS\_QUANTITY)

**Examples**

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

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

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

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

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

```

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

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

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

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

```

guess\_sep

*Guess separator***Description**

Guess separator

**Usage**

```

guess_sep(x, ...)

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

## S3 method for class 'factor'
guess_sep(x, ...)

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

```

**Arguments**

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

**Value**

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

## Examples

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

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

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

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

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

**impute\_systematic\_nondetects**  
*Impute systematic nondetects*

## Description

Impute systematic nondetects

## Usage

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

## Arguments

object	SummarizedExperiment
subgroup	subgroup svar
fun	imputation function
plot	TRUE or FALSE
verbose	TRUE or FALSE
...	passed to ‘fun’

**Value**

SummarizedExperiment

**Examples**

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

---

invert

*Invert*

---

**Description**

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

**Usage**

```
invert(x, ...)

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

## S3 method for class 'SummarizedExperiment'
invert(
  x,
  subgroups = slevels(x, "subgroup"),
  sep = guess_sep(x, "subgroup"),
  ...
)
```

**Arguments**

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

**Value**

character vector or SummarizedExperiment

## Examples

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

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

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

## Description

Get/Set is\_imputed

## Usage

```
is_imputed(object)

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

is_imputed(object) <- value

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

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

## Arguments

object	SummarizedExperiment
value	matrix

## Value

matrix (get) or updated object (set)

## Examples

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

---

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

---

## Description

Is significant?

## Usage

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

## Arguments

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

## Value

matrix: -1 (downregulated), +1 (upregulated), 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**      *Get/Set log2countsratios*

## 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_rnasedq_counts(file, plot=FALSE)
log2countsratios(object) <- values(object)
log2countsratios(object)[1:3, 1:3]
```

---

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

---

## Description

Get / Set log2cpm matrix

## Usage

```
log2cpm(object)

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

log2cpm(object) <- value

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

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

## Arguments

object	SummarizedExperiment
value	log2cpm matrix (features x samples)

## Value

log2cpm matrix (get) or updated object (set)

## Examples

```
file <- download_data('billig19.rnacounts.txt')
object <- read_rnaseq_counts(file, plot=FALSE)
log2cpm(object) <- values(object)
log2cpm(object)[1:3, 1:3]
```

`log2cpmratios`      *Get/Set log2cpmratios*

## 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

<code>object</code>	SummarizedExperiment
<code>value</code>	<code>log2cpmratios</code> matrix (features x samples)

## Value

`log2cpmratios` matrix (get) or updated object (set)

## Examples

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

---

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

---

## Description

Get / Set log2tpm matrix

## Usage

```
log2tpm(object)

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

log2tpm(object) <- value

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

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

## Arguments

object	SummarizedExperiment
value	log2tpm matrix (features x samples)

## Value

log2tpm matrix (get) or updated object (set)

## Examples

```
file <- download_data('billig19.rnacounts.txt')
object <- read_rnaseq_counts(file, plot=FALSE)
log2tpm(object) <- values(object)
log2tpm(object)[1:3, 1:3]
```

`log2tpmratios`      *Get/Set log2tpmratios*

## 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	<code>log2tpmratios</code> matrix (features x samples)

## Value

`log2tpmratios` matrix (get) or updated object (set)

## Examples

```
file <- download_data('billing19.rnacounts.txt')
object <- read_rnasedq_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()
zscore(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

<code>object</code>	SummarizedExperiment
<code>fit</code>	'limma', 'lme', 'lm', 'wilcoxon'
<code>contrastdefmat</code>	contrastdef matrix
<code>ntop</code>	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)
```

**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
```

*maxquant quantity patterns*

---

**Description**

maxquant quantity patterns

**Usage**

```
MAXQUANT_PATTERNS_QUANTITY
```

**Format**

An object of class character of length 7.

**Examples**

```
MAXQUANT_PATTERNS_QUANTITY
```

---

```
merge_sdata
```

*Merge sample/feature data*

---

**Description**

Merge sample/feature data

**Usage**

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

**Arguments**

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

**Value**

SummarizedExperiment

**Examples**

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

---

merge\_sfile

*Merge sample/feature file*

---

**Description**

Merge sample/feature file

**Usage**

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

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

**Arguments**

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

**Value**

SummarizedExperiment

**Examples**

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

---

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

---

**Description**

message dataframe using sprintf syntax. Use place holder '

**Usage**

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

**Arguments**

format_string	sprintf style format string
x	data.frame

**Value**

nothing returned

**Examples**

```
x <- data.frame(feature_id = c('F001', 'F002'), symbol = c('FEAT1', 'FEAT2'))  
message_df('\t%s', x)  
  
x <- c(rep('PASS', 25), rep('FAIL', 25))  
message_df(format_string = '%s', table(x))
```

---

---

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

---

**Description**

stri\_split and extract

**Usage**

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

**Arguments**

x	string
sep	string
i	integer

**Value**

character

**Examples**

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

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

**normimpute**

*Impute from half-normal distribution around 0*

**Description**

Impute from half-normal distribution around 0

**Usage**

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

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

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

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

**Arguments**

<b>x</b>	NA-containing numeric vector
<b>selector</b>	which values to impute
<b>mean</b>	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      *Plot sample/feature boxplots*

---

**Description**

Plot sample/feature boxplots

**Usage**

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

```

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

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

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

```

### Arguments

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

### Value

ggplot object

### See Also

[plot\\_sample\\_densities](#), [plot\\_sample\\_violins](#)

## Examples

```
# data
  require(magrittr)
  file <- download_data('halama18.metabolon.xlsx')
  object <- read_metabolon(file, plot = FALSE)
  object %>% extract(, order(.\$Group))
  fdata(object) %>% cbind(
    control = .\$feature_name %in% c('biotin', 'phosphate'))
# plot
  plot_boxplots(object[1:9], x = feature_id, fill = feature_id)
  plot_boxplots(object[, 1:9], x = sample_id, fill = sample_id)
  plot_feature_boxplots(object[1:9, ])
  plot_sample_boxplots(object[, 1:12])
  plot_sample_boxplots(object[, 1:12], highlight = control)
  plot_subgroup_boxplots(object[1:2, ], subgroup = Group)
```

`plot_contrastogram`      *Plot contrastogram*

## Description

Plot contrastogram

## Usage

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

## Arguments

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

## Value

list returned by [plotmat](#)

## Examples

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

**plot\_corrections**      *Biplot batch corrections*

## Description

Biplot batch corrections

## Usage

```
plot_corrections(...)

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

## Arguments

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

## Value

grid object

## See Also

[biplot\\_covariates](#)

## Examples

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

---

plot\_covariates      *Biplot covariates*

---

## Description

Biplot covariates

## Usage

```
plot_covariates(...)

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

## Arguments

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

## Value

ggplot object

## See Also

biplot\_corrections

## Examples

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

**plot\_data**

*Plot data*

## Description

Plot data

## Usage

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

## Arguments

<code>data</code>	<code>data.frame'</code>
<code>geom</code>	<code>geom_point</code> , etc.
<code>color</code>	variable mapped to color (symbol)
<code>fill</code>	variable mapped to fill (symbol)
<code>...</code>	mapped aesthetics
<code>fixed</code>	fixed aesthetics (list)
<code>theme</code>	list with ggplot theme specifications

## Value

ggplot object

## Author(s)

Aditya Bhagwat, Johannes Graumann

## Examples

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

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

---

plot\_densities      *Plot sample/feature densities*

---

## Description

Plot sample/feature densities

## Usage

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

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

plot_feature_densities(
  object,
  fill = feature_id,
  color = NULL,
  group = feature_id,
```

```

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

```

### Arguments

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

### Value

ggplot object

### See Also

[plot\\_sample\\_violins](#), [plot\\_sample\\_boxplots](#)

### Examples

```

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

```

### 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 a 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

<code>object</code>	SummarizedExperiment
<code>geom</code>	geom_point, geom_boxplot, etc.
<code>subgroup</code>	subgroup svar
<code>x</code>	svar mapped to x
<code>fill</code>	svar mapped to fill
<code>color</code>	svar mapped to color
<code>...</code>	mapped aesthetics
<code>fixed</code>	fixed aesthetics
<code>theme</code>	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

*Plot venn*

---

## 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`      *Plot sample/feature violins*

---

## Description

Plot sample/feature violins

## Usage

```
plot_violins(  
  object,  
  x,  
  fill,  
  color = NULL,  
  group = NULL,  
  facet = NULL,  
  highlight = NULL,  
  fixed = list(na.rm = TRUE)  
)  
  
plot_sample_violins(  
  object,  
  x = sample_id,  
  fill = sample_id,  
  color = NULL,  
  highlight = NULL,  
  fixed = list(na.rm = TRUE)  
)  
  
plot_feature_violins(  
  object,  
  x = feature_id,  
  fill = feature_name,  
  color = NULL,  
  highlight = NULL,  
  fixed = list(na.rm = TRUE)  
)  
  
plot_subgroup_violins(  
  object,  
  subgroup,  
  x = !!enquo(subgroup),  
  fill = !!enquo(subgroup),  
  color = NULL,  
  highlight = NULL,  
  facet = feature_id,  
  fixed = list(na.rm = TRUE)
```

)

### Arguments

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

### Value

ggplot object

### See Also

[plot\\_sample\\_densities](#), [plot\\_sample\\_boxplots](#)

### Examples

```
# data
  require(magrittr)
  file <- download_data('halama18.metabolon.xlsx')
  object <- read_metabolon(file, plot = FALSE)
  object %>% extract(, order(.Group))
  control_features <- c('biotin', 'phosphate')
  fdata(object) %>% cbind(control=.feature_name %in% control_features)
# plot
  plot_violins(object[1:12, ], x=feature_id, fill=feature_id)
  plot_feature_violins(object[1:12, ])
  plot_sample_violins(object[, 1:12], highlight = control)
  plot_subgroup_violins(object[1:4, ], subgroup = Group)
```

---

plot\_volcano

*Plot volcano*

---

### Description

Plot volcano

**Usage**

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

**Arguments**

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

**Value**

ggplot object

**Examples**

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

**preprocess\_rnaseq\_counts**

*Preprocess RNAseq counts*

**Description**

Preprocess RNAseq counts

**Usage**

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

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

**Arguments**

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

**Value**

SummarizedExperiment

**Examples**

```
require(magrittr)  
file <- download_data('billig19.rnacounts.txt')  
object <- .read_rnaseq_counts(file)  
object$subgroup  
object %>>% preprocess_rnaseq_counts()
```

---

**proteingroups**      *Get/Set proteingroups*

---

**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**      *Read affymetrix microarray*

**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** *Get tmm-scaled libsizes*

### Description

Get tmm-scaled libsizes

### Usage

```
scaledlibsizes(counts)
```

### Arguments

counts	counts matri
--------	--------------

### 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** *Get/Set sdata*

### Description

Get/Set sample data

### Usage

```
sdata(object)

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

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

sdata(object) <- value

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

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

### Arguments

object	SummarizedExperiment, eSet, or EList
value	dataframe

### Value

sample dataframe (get) or updated object (set)

### Examples

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

---

## slevels

*Get slevels*

---

### Description

Get svar levels

### Usage

```
slevels(object, svar)  
  
subgroup_levels(object)
```

### Arguments

object	SummarizedExperiment, eSet, or EList
svar	sample var (character)

### Value

svar values (character)

## Examples

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

*snames*

*Get/Set snames*

## Description

Get/Set sample names

## Usage

```
snames(object)

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

snames(object) <- value

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

## Arguments

object	SummarizedExperiment
value	string vector with sample names

## Value

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

## Examples

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

---

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

---

**Description**

Split by svar

**Usage**

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

**Arguments**

object	SummarizedExperiment
svar	svar to split on

**Value**

list of SummarizedExperiment

**Examples**

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

---

---

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

---

**Description**

Standardize maxquant sample names

**Usage**

```
standardize_maxquant_snames(x, ...)

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

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

## Arguments

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

## Details

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

## Value

character vector or SummarizedExperiment

## Examples

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

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

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

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

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

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

---

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

---

**Description**

Arrange (subgroup)levels in matrix

**Usage**

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

**Arguments**

object	SummarizedExperiment
subgroupvar	subgroup svar

**Value**

matrix

**Examples**

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

---

---

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

---

**Description**

Subtract baseline level within block

**Usage**

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

```

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

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

```

## Arguments

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

## Details

*subtract\_baseline* subtracts baseline levels within block, using the medoid baseline sample if multiple exist.

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

*subtract\_differences* subtracts differences between subsequent levels, again within block

## Value

SummarizedExperiment

## Examples

```

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

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

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

```

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

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

---

**sumexp2mae***Create MultiAssayExperiment from SummarizedExperiment list*

---

## Description

Create MultiAssayExperiment from SummarizedExperiment list

## Usage

```
sumexp2mae(experiments)
```

## Arguments

`experiments`      named list of SummarizedExperiments

## Value

MultiAssayExperiment

## Examples

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

**sumexp\_to\_wide\_dt**      *Convert SummarizedExperiment into data.table*

## Description

Convert SummarizedExperiment into data.table

## Usage

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

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

sumexp_to_subrep_dt(object, subgroup = subgroup)
```

## Arguments

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

## Details

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

## Value

data.table

## Examples

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

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

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

summarize\_fit

*Summarize fit*

## Description

Summarize fit

## Usage

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

## Arguments

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

## Value

```
data.table(contrast, nup, ndown)
```

## Examples

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

**svalues**

*Get/Set svalues*

## Description

Get/Set svar values

## Usage

```
svalues(object, svar)

subgroup_values(object)

sampleid_values(object)

svalues(object, svar) <- value

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

## Arguments

object	SummarizedExperiment
svar	sample var (character)
value	value vector

## Value

character vector (get) or SummarizedExperiment (set)

## Examples

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

---

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

---

## Description

Get/Set sample variables

## Usage

```
svars(object)

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

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

svars(object) <- value

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

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

## Arguments

object	SummarizedExperiment
value	string factor with variable names

## Value

sample variable names (get) or updated SummarizedExperiment

## Examples

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

TESTS

*Statistical models supported in autonomics***Description**

Statistical models supported in autonomics

**Usage**

TESTS

**Format**

An object of class character of length 5.

**Examples**

TESTS

**tpm***Get/Set tpm***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_rnased_counts(file, plot=FALSE)
tpm(object) <- values(object)
tpm(object)[1:3, 1:3]
```

---

values	<i>Get/Set expr values</i>
--------	----------------------------

---

**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]
```

100

*weights*

---

venn\_detects

*Venn detects*

---

### Description

Venn diagram full/systematic/random detects

### Usage

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

### Arguments

object	SummarizedExperiment
subgroup	subgroup symbol

### Value

```
NULL
```

### Examples

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

---

weights

*Get/Set weights*

---

### Description

Get/Set weight matrix

### Usage

```
weights(object, ...)

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

weights(object) <- value

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

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

```

weights(object) <- value

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

```

**Arguments**

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

**Value**

weight matrix (get) or updated object (set)

**Examples**

```

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

```

zero\_to\_na

*Change nondetect representation***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\_PEPCOUNTS, 61  
MAXQUANT\_PATTERNS\_QUANTITY, 62  
TESTS, 98  
.read\_maxquant, 4  
.read\_metabolon, 6  
.read\_rectangles, 8  
.read\_rnaseq\_bams, 11  
.read\_rnaseq\_counts  
  (.read\_rnaseq\_bams), 11  
.read\_somascan, 14  
  
add\_smiles, 15  
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, 19  
biplot\_corrections (plot\_corrections),  
  72  
biplot\_covariates (plot\_covariates), 73  
  
center, 20  
contrast\_subgroup\_cols, 22  
contrast\_subgroup\_rows  
  (contrast\_subgroup\_cols), 22  
contrastdefs, 21  
contrastdefs, SummarizedExperiment-method  
  (contrastdefs), 21  
contrastdefs<- (contrastdefs), 21  
contrastdefs<-, SummarizedExperiment, list-method  
  (contrastdefs), 21  
counts, 23  
  
counts, SummarizedExperiment-method  
  (counts), 23  
counts2cpm, 24  
counts2tpm, 24  
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, 27  
default\_subgroupvar, 28  
download\_data, 29  
download\_gtf, 30  
dt2mat, 31  
  
exp2 (log2transform), 59  
explore\_imputations, 31  
explore\_transformations, 32  
extract\_features, 33  
extract\_rectangle, 34  
  
fdata, 36  
fdata, SummarizedExperiment-method  
  (fdata), 36

```

fdata<- (fdata), 36
fdata<-, SummarizedExperiment,data.frame-method limma, SummarizedExperiment-method
    (fdata), 36
filter_exprs_replicated_in_some_subgroup, limma<- (limma), 52
    37
filter_features, 38
filter_medoid, 38
filter_replicated, 39
filter_samples, 40
fit_limma, 40
fit_lm(fit_limma), 40
fit_lme(fit_limma), 40
fit_lmer(fit_limma), 40
fit_wilcoxon(fit_limma), 40
flevels, 42
fnames, 43
fnames, SummarizedExperiment-method
    (fnames), 43
fnames<- (fnames), 43
fnames<-, SummarizedExperiment,character-method
    (fnames), 43
formula2str, 44
fvalues, 44
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<- (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

```

(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\_PEPCOUNTS, 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  
quantnorm (log2transform), 59  
pca, 68  
plot\_biplot (biplot), 19  
plot\_boxplots, 69  
plot\_contrastogram, 71  
plot\_corrections, 72  
plot\_covariates, 73  
plot\_data, 74  
plot\_densities, 75  
plot\_detections (plot\_detects), 76  
plot\_detects, 76  
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\_idfeatures, 78  
plot\_quantifications (plot\_detects), 76  
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), 76  
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  
quartnorm (log2transform), 59  
read\_affymetrix, 84  
read\_metabolon (.read\_metabolon), 6  
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