Package 'autonomics'

July 2, 2025

Type Package

Title Unified Statistical Modeling of Omics Data

Version 1.16.0

Description This package unifies access to Statistal Modeling of Omics Data.
Across linear modeling engines (lm, lme, lmer, limma, and wilcoxon).
Across coding systems (treatment, difference, deviation, etc).
Across model formulae (with/without intercept, random effect, interaction or nesting).
Across omics platforms (microarray, rnaseq, msproteomics, affinity proteomics, metabolomics).
Across projection methods (pca, pls, sma, lda, spls, opls).
Across clustering methods (hclust, pam, cmeans).
It provides a fast enrichment analysis implementation.
And an intuitive contrastogram visualisation to summarize contrast effects in complex designs.

License GPL-3

Encoding UTF-8

LazyData true

VignetteBuilder knitr

biocViews Software, DataImport, Preprocessing, DimensionReduction,
PrincipalComponent, Regression, DifferentialExpression,
GeneSetEnrichment, Transcriptomics, Transcription,
GeneExpression, RNASeq, Microarray, Proteomics, Metabolomics,
MassSpectrometry,

BugReports
https://gitlab.uni-marburg.de/fb20/ag-graumann/software/autonomics/issues

RoxygenNote 7.3.1

Depends R (>= 4.0)

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ggplot2, ggrepel, graphics, grDevices, grid, gridExtra, limma,
magrittr, matrixStats, methods, MultiAssayExperiment, parallel,
RColorBrewer, rlang, R.utils, readxl, S4Vectors, scales, stats,
stringi, SummarizedExperiment, survival, tidyr, tidyselect,
tools, utils, vsn

Suggests affy, AnnotationDbi, AnnotationHub, apcluster, Biobase, BiocManager, BiocStyle, Biostrings, coin, diagram, DBI, e1071, ensembldb, GenomicDataCommons, GenomicRanges, GEOquery, ggtext, hgu95av2.db, ICSNP, jsonlite, knitr, lme4, lmerTest, MASS, patchwork, mixOmics, mpm, nlme, OlinkAnalyze, org.Hs.eg.db, org.Mm.eg.db, pcaMethods, pheatmap, progeny, propagate, RCurl, RSQLite, remotes, rmarkdown, ropls, Rsubread, readODS, rtracklayer, statmod, testthat, UniProt.ws, writexl, XML

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Contents

.coxph *Fit onefeature survival*

Description

Fit onefeature survival

Usage

```
.coxph(timetoevent, event, expr)

.survdiff(timetoevent, event, expr)

.logrank(timetoevent, event, expr)
```

Arguments

timetoevent	numeric (time to event)
event	numeric (1=event, 0=not)
expr	numeric (.coxph) or twolevel-factor (.survdiff, .logrank_test)

Examples

```
# Prepare
         object <- survival_example()
    timetoevent <- object$timetoevent
          event <- object$event
           expr <- values(object)[1,]
       quantile <- factor(dplyr::ntile(expr, 2))
# Survival
       .coxph(timetoevent, event, expr)
    .survdiff(timetoevent, event, quantile)
     .logrank(timetoevent, event, quantile)
# Sumexp
         fit_survival(object)
```

.extract_p_features *Extract coefficient features*

Description

Extract coefficient features

Usage

```
.extract_p_features(
  object,
  coefs,
  p = 0.05,
  fit = fits(object),
  combiner = "|",
  features = NULL,
  verbose = TRUE
)

.extract_fdr_features(
  object,
  coefs,
  fdr = 0.05,
  fit = fits(object),
  combiner = "|",
  features = NULL,
  verbose = TRUE
)

.extract_effectsize_features(
  object,
  coefs,
  effectsize = 1,
  fit = fits(object),
  combiner = "|",
  features = NULL,
  verbose = TRUE
)

.extract_sign_features(
  object,
  coefs,
  sign,
  fit = fits(object)[1],
  combiner = "|",
  features = NULL,
  verbose = TRUE
)

.extract_n_features(
  object,
  coefs,
  combiner = "|",
  n,
  fit = fits(object)[1],
  features = NULL,
```

```
  verbose = TRUE
)

extract_coef_features(
  object,
  fit = fits(object)[1],
  coefs = autonomics::coefs(object, fit = fit),
  combiner = "|",
  decreasing = FALSE,
  p = 1,
  fdr = 1,
  effectsize = 0,
  sign = c(-1, +1),
  n = 4,
  features = NULL,
  verbose = TRUE
)
```

Arguments

object	SummarizedXExperiment
coefs	subset of coefs(object)
p	p threshold
fit	subset of fits(object)
combiner	'|' or '&': how to combine multiple fits/coefs
features	features to include no matter what (character vector)
verbose	TRUE or FALSE
fdr	fdr threshold
effectsize	effectsize threshold
sign	effect sign
n	number of top features (Inf means all)
decreasing	TRUE or FALSE

Value

SummarizedExperiment

Examples

```
# Read and Fit
    file <- system.file('extdata/atkin.metabolon.xlsx', package = 'autonomics')
    object <- read_metabolon(file)
    object %<>% fit_limma()
    fdt(object) %<>% add_adjusted_pvalues('fdr')
# Single coef
    object0 <- object
```

```
    object %<>% .extract_p_features(         coefs = 't1-t0', p = 0.05)
    object %<>% .extract_fdr_features(       coefs = 't1-t0', fdr = 0.05)
    object %<>% .extract_effectsize_features(coefs = 't1-t0', effectsize = 1)
    object %<>% .extract_sign_features(      coefs = 't1-t0', sign = -1)
    object %<>% .extract_n_features(         coefs = 't1-t0', n = 1)
    object <- object0
    object %<>%  extract_coef_features(
                 coefs = 't1-t0', p = 0.05, fdr = 0.05, effectsize = 1, sign = -1, n = 1)
# Multiple coefs
    object <- object0
    object %<>% .extract_p_features(         coefs = c('t1-t0', 't2-t0'), p = 0.05)
    object %<>% .extract_fdr_features(       coefs = c('t1-t0', 't2-t0'), fdr = 0.01)
    object %<>% .extract_effectsize_features(coefs = c('t1-t0', 't2-t0'), effectsize = 1)
    object %<>% .extract_sign_features(      coefs = c('t1-t0', 't2-t0'), sign = -1)
    object %<>% .extract_n_features(         coefs = c('t1-t0', 't2-t0'), n = 1)
    object <- object0
    object %<>%  extract_coef_features(
             coefs = c('t1-t0', 't2-t0'), p = 0.05, fdr = 0.01, effectsize = 1, sign = -1, n = 1)
```

`.merge` *Clean Merge*

Description

Clean Merge

Usage

```
.merge(dt1, dt2, by)
```

Arguments

`dt1`	data.table
`dt2`	data.table
`by`	string

Examples

```
require(data.table)
dt1 <- data.table(feature_id = c('PG1', 'PG2'), gene    = c('G1', 'G2'))
dt2 <- data.table(feature_id = c('PG1', 'PG2'), protein = c('P1', 'P2'))
dt1 %<>% .merge(dt2, by = 'feature_id')
dt1
```

.read_compounddiscoverer

Read compound discoverer files as-is

Description

Read compound discoverer files as-is

Usage

```
.read_compounddiscoverer(
  file,
  quantity = guess_compounddiscoverer_quantity(file),
  colname_format = NULL,
  mod_extract = NULL,
  verbose = TRUE
)
```

Arguments

file	compoumd discoverer file
quantity	string
colname_format	function to reformat column names
mod_extract	function to extract MS modi from sample names
verbose	TRUE / FALSE

Value

data.table

.read_compounddiscoverer_masslist

Read compound discoverer masslist files as-is

Description

Read compound discoverer masslist files as-is

Usage

```
.read_compounddiscoverer_masslist(file, verbose = TRUE)
```

Arguments

file	compoumd discoverer masslist file
verbose	TRUE / FALSE

Value

data.table

.read_diann_precursors *Read diann*

Description

Read diann

Usage

```
.read_diann_precursors(file, Lib.PG.Q = 0.01, verbose = TRUE)

.read_diann_proteingroups(file, Lib.PG.Q = 0.01)

read_diann_proteingroups(
  file,
  Lib.PG.Q = 0.01,
  simplify_snames = TRUE,
  rm_contaminants = TRUE,
  impute = FALSE,
  plot = FALSE,
  pca = plot,
  pls = plot,
  fit = if (plot) "limma" else NULL,
  formula = as.formula("~ subgroup"),
  block = NULL,
  coefs = NULL,
  contrasts = NULL,
  palette = NULL,
  verbose = TRUE
)

read_diann(...)
```

Arguments

file	'report.tsv' file
Lib.PG.Q	Lib.PG.Q cutoff

verbose	TRUE or FALSE
simplify_snames	TRUE or FALSE: simplify (drop common parts in) samplenames ?
rm_contaminants	TRUE or FALSE: rm contaminants ?
impute	TRUE or FALSE: impute group-specific NA values ?
plot	TRUE or FALSE
pca	TRUE or FALSE: run pca ?
pls	TRUE or FALSE: run pls ?
fit	model engine: 'limma', 'lm', 'lme(r)', 'wilcoxon' or NULL
formula	model formula
block	model blockvar: string or NULL
coefs	model coefficients of interest: character vector or NULL
contrasts	coefficient contrasts of interest: character vector or NULL
palette	color palette: named string vector
...	used to maintain deprecated functions

Value

data.table or SummarizedExperiment

Examples

```
# Read
   file <- download_data('dilution.report.tsv')
   .read_diann_precursors(file)         #    precursors longdt
   .read_diann_proteingroups(file)      # proteingroups longdt
   fdt(read_diann_proteingroups(file))  # proteingroups sumexp
# Compare
    PR <- .read_diann_precursors(file)
    PG <- .read_diann_proteingroups(file)
    PG[intensity==top1] # matches      : 24975 (85%) proteingroups
    PG[intensity!=top1] # doesnt match :  4531 (15%) proteingroups
    RUN <- 'IPT_HeLa_1_DIAstd_Slot1-40_1_9997'
    PR[uniprot=='Q96JP5;Q96JP5-2' & run == RUN, 1:6] #    match:    8884 ==   8884
    PR[uniprot=='P36578'          & run == RUN, 1:6] # no match:  650887 != 407978
  PR[intensity != top1][feature_id == unique(feature_id)[1]][run == unique(run)[1]][1:2, 1:6]
  PR[intensity != top1][feature_id == unique(feature_id)[2]][run == unique(run)[1]][1:2, 1:6]
  PR[intensity != top1][feature_id == unique(feature_id)[3]][run == unique(run)[1]][1:3, 1:6]
```

.read_maxquant_proteingroups *Read proteingroups/phosphosites as-is*

Description

Read proteingroups/phosphosites as-is

Usage

```
.read_maxquant_proteingroups(
  file,
  quantity = guess_maxquant_quantity(file),
  verbose = TRUE
)

.read_maxquant_phosphosites(
  file,
  profile,
  quantity = guess_maxquant_quantity(file),
  verbose = TRUE
)
```

Arguments

file	proteingroups / phosphosites file
quantity	string
verbose	TRUE / FALSE
profile	proteingroups file

Value

data.table

Examples

```
profile <- system.file('extdata/billing19.proteingroups.txt', package = 'autonomics')
fosfile <- system.file('extdata/billing19.phosphosites.txt',  package = 'autonomics')
prodt <- .read_maxquant_proteingroups(file = profile)
fosdt <- .read_maxquant_phosphosites( file = fosfile, profile = profile)
```

`.read_metabolon` *Read metabolon xlsxfile*

Description

Read metabolon xlsxfile

Usage

```
.read_metabolon(
  file,
  sheet = "OrigScale",
  fidvar = "BIOCHEMICAL",
  sidvar = "(CLIENT_IDENTIFIER|Client ID)",
  sfile = NULL,
  by.x = "sample_id",
  by.y = NULL,
  groupvar = NULL,
  verbose = TRUE
)

read_metabolon(
  file,
  sheet = "OrigScale",
  fidvar = "BIOCHEMICAL",
  sidvar = "(CLIENT_IDENTIFIER|Client ID)",
  sfile = NULL,
  by.x = "sample_id",
  by.y = NULL,
  groupvar = NULL,
  fnamevar = "BIOCHEMICAL",
  kegg_pathways = FALSE,
  smiles = FALSE,
  impute = TRUE,
  plot = FALSE,
  pca = plot,
  pls = plot,
  label = "feature_id",
  fit = if (plot) "limma" else NULL,
  formula = as.formula("~ subgroup"),
  block = NULL,
  coefs = NULL,
  contrasts = NULL,
  palette = NULL,
  verbose = TRUE
)
```

Arguments

file	metabolon xlsx file
sheet	excel sheet (number or string)
fidvar	featureid var
sidvar	samplid var
sfile	sample file
by.x	‘file‘ mergeby column
by.y	‘sfile‘ mergeby column
groupvar	string
verbose	TRUE or FALSE
fnamevar	featurename fvar
kegg_pathways	TRUE or FALSE: add kegg pathways?
smiles	TRUE or FALSE: add smiles?
impute	TRUE or FALSE: impute group-specific NA values?
plot	TRUE or FALSE
pca	TRUE or FALSE
pls	TRUE or FALSE
label	fvar
fit	model engine: ’limma’, ’lm’, ’lme(r)’, ’wilcoxon’ or NULL
formula	model formula
block	model blockvar: string or NULL
coefs	model coefficients of interest: character vector or NULL
contrasts	coefficient contrasts of interest: character vector or NULL
palette	NULL or colorvector

Value

SummarizedExperiment

Examples

```
file <- system.file('extdata/atkin.metabolon.xlsx', package = 'autonomics')
read_metabolon(file, plot = TRUE, block = 'Subject')
```

`.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 <- system.file('extdata/billing19.rnacounts.txt', package = 'autonomics')
   read_rectangles( file, fid_rows = 2:25,     fid_cols = 2,
                          sid_rows = 1,        sid_cols = 5:28,
                         expr_rows = 2:25 ,   expr_cols = 5:28,
                         fvar_rows = 1,       fvar_cols = 1:4,
                        fdata_rows = 2:25 ,  fdata_cols = 1:4,   transpose = FALSE)
```

```
# LCMSMS PROTEINGROUPS
   file <- system.file('extdata/billing19.proteingroups.txt', package = 'autonomics')
   read_rectangles(  file,
                     fid_rows = 2:21,    fid_cols = 383,
                     sid_rows = 1,       sid_cols = seq(124, 316, by = 6),
                    expr_rows = 2:21,   expr_cols = seq(124, 316, by = 6),
                     fvar_rows = 1,      fvar_cols = c(2, 6, 7, 383),
                   fdata_rows = 2:21,  fdata_cols = c(2, 6, 7, 383),
                   transpose  = FALSE )
# SOMASCAN
   file <- system.file('extdata/atkin.somascan.adat', package = 'autonomics')
   read_rectangles(file, fid_rows = 30,         fid_cols = 23:42,
                         sid_rows = 42:108,     sid_cols = 4,
                        expr_rows = 42:108,    expr_cols = 23:42,
                        fvar_rows = 28:40,     fvar_cols = 22,
                        svar_rows = 41,        svar_cols = 1:21,
                       fdata_rows = 28:40,    fdata_cols = 23:42,
                       sdata_rows = 42:108,   sdata_cols = 1:21,  transpose  = TRUE)
# METABOLON
   file <- system.file('extdata/atkin.metabolon.xlsx', package = 'autonomics')
   read_rectangles(file, sheet = 2,
                     fid_rows = 11:30,     fid_cols = 2,
                     sid_rows = 4,         sid_cols = 15:81,
                    expr_rows = 11:30,    expr_cols = 15:81,
                     fvar_rows = 10,       fvar_cols = 1:14,
                     svar_rows = 1:10,     svar_cols = 14,
                   fdata_rows = 11:30,   fdata_cols = 1:14,
                   sdata_rows = 1:10,    sdata_cols = 15:81,
                    transpose = FALSE )
```

`.read_rnaseq_bams` *Read rnaseq counts/bams*

Description

Read rnaseq counts/bams

Usage

```
.read_rnaseq_bams(
  dir,
  paired,
  genome,
  nthreads = detectCores(),
  sfile = NULL,
  by.y = NULL,
  ensdb = NULL,
  verbose = TRUE
)
```

```
.read_rnaseq_counts(
  file,
  fid_col = 1,
  sfile = NULL,
  by.y = NULL,
  ensdb = NULL,
  verbose = TRUE
)

read_rnaseq_bams(
  dir,
  paired,
  genome,
  nthreads = detectCores(),
  sfile = NULL,
  by.y = NULL,
  block = NULL,
  formula = as.formula("~ subgroup"),
  min_count = 10,
  pseudo = 0.5,
  ensdb = NULL,
  tpm = FALSE,
  cpm = TRUE,
  log2 = TRUE,
  plot = FALSE,
  label = "feature_id",
  pca = plot,
  pls = plot,
  fit = if (plot) "limma" else NULL,
  voom = cpm,
  coefs = NULL,
  contrasts = NULL,
  palette = NULL,
  verbose = TRUE
)

read_rnaseq_counts(
  file,
  fid_col = 1,
  sfile = NULL,
  by.y = NULL,
  formula = as.formula("~ subgroup"),
  block = NULL,
  min_count = 10,
  pseudo = 0.5,
  tpm = FALSE,
  ensdb = NULL,
```

```
  cpm = !tpm,
  log2 = TRUE,
  plot = FALSE,
  label = "feature_id",
  pca = plot,
  pls = plot,
  fit = if (plot) "limma" else NULL,
  voom = cpm,
  coefs = NULL,
  contrasts = NULL,
  palette = NULL,
  verbose = TRUE
)
```

Arguments

dir	read_rnaseq_bams: bam/sam dir
paired	read_rnaseq_bams: TRUE/FALSE : paired end reads ?
genome	read_rnaseq_bams: 'mm10', 'hg38', etc. or GTF file
nthreads	read_rnaseq_bams: nthreads used by Rsubread::featureCounts()
sfile	sample file
by.y	sample file mergeby column
ensdb	EnsDb with genesizes : e.g. AnnotationHub::AnnotationHub[['AH64923']]
verbose	TRUE or FALSE: message?
file	count file
fid_col	featureid column (number or string)
block	model blockvar: string or NULL
formula	model formula
min_count	min feature count required in some samples
pseudo	pseudocount added to prevent -Inf log2 values
tpm	TRUE or FALSE : add tpm to assays (counts / libsize / genelength) ?
cpm	TRUE or FALSE: add cpm to assays (counts / effectivelibsize) ?
log2	TRUE or FALSE: log2 transform ?
plot	TRUE or FALSE: plot?
label	fvar
pca	TRUE or FALSE: perform and plot pca?
pls	TRUE or FALSE: run pls ?
fit	model engine: 'limma', 'lm', 'lme(r)', 'wilcoxon' or NULL
voom	model weights to be computed? TRUE/FALSE
coefs	model coefficients of interest: string vector or NULL
contrasts	model coefficient contrasts of interest: string vector or NULL
palette	color palette : named string vector

Value

SummarizedExperiment

Author(s)

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Examples

```
# read_rnaseq_bams
  if (requireNamespace('Rsubread')){
      dir <- download_data('billing16.bam.zip')
      object <- read_rnaseq_bams(dir, paired = TRUE, genome = 'hg38')
      object <- read_rnaseq_bams(dir, paired = TRUE, genome = 'hg38', plot = TRUE)
  }
# read_rnaseq_counts
  file <- system.file('extdata/billing19.rnacounts.txt', package = 'autonomics')
  object <- read_rnaseq_counts(file, fit = 'limma', coefs = 'E15-E00')
  object <- read_rnaseq_counts(file, fit = 'limma', coefs = 'E15-E00', voom = FALSE)
 object <- read_rnaseq_counts(file, fit = 'limma', coefs = 'E15-E00', voom = FALSE, cpm = FALSE)
 object <- read_rnaseq_counts(file, fit = 'limma', coefs = 'E15-E00', voom = FALSE, cpm = FALSE,
                                    log2 = FALSE)
  object <- read_rnaseq_counts(file, plot = TRUE)

# read_rnaseq_counts(tpm = TRUE)
  ## Not run:
  ah <- AnnotationHub::AnnotationHub()
  ensdb <- ah[['AH64923']]
 object <- read_rnaseq_counts(file, fit = 'limma', coefs = 'E02-E00', tpm = TRUE, ensdb = ensdb)

## End(Not run)
```

.read_somascan *Read somascan adatfile*

Description

Read somascan adatfile

Usage

```
.read_somascan(
  file,
  fidvar = "Target",
  sidvar = "SampleId",
  sfile = NULL,
  by.x = NULL,
  by.y = NULL,
  groupvar = "SampleGroup",
```

```
  verbose = TRUE
)

read_somascan(
  file,
  fidvar = "Target",
  sidvar = "SampleId",
  sfile = NULL,
  by.x = NULL,
  by.y = NULL,
  groupvar = "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,
  plot = FALSE,
  label = "feature_id",
  pca = plot,
  pls = plot,
  fit = if (plot) "limma" else NULL,
  formula = as.formula(sprintf("~ %s", groupvar)),
  block = NULL,
  coefs = NULL,
  contrasts = NULL,
  palette = NULL,
  verbose = TRUE
)
```

Arguments

file	somascan (adat) file
fidvar	featureid var
sidvar	sampleid var
sfile	sample file
by.x	‘file‘ mergeby column
by.y	‘sfile‘ mergeby column
groupvar	string
verbose	TRUE or FALSE: message?
fname_var	featurename var: 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	TRUE or FALSE: rm NA svars?
rm_single_value_svars	TRUE or FALSE: rm single value svars?
plot	TRUE or FALSE: plot ?
label	fvar
pca	TRUE or FALSE: run pca?
pls	TRUE or FALSE: run pls?
fit	model engine: 'limma', 'lm', 'lme(r)','wilcoxon' or NULL
formula	model formula
block	model blockvar
coefs	model coefficients of interest: character vector or NULL
contrasts	coefficient contrasts of interest: character vector or NULL
palette	character vector or NULL

Value

Summarizedexperiment

Examples

```
file <- system.file('extdata/atkin.somascan.adat', package = 'autonomics')
read_somascan(file, plot = TRUE, block = 'Subject')
```

---

abstract_fit *Abstract model fit*

Description

Abstract model fit

Usage

```
abstract_fit(
  object,
  sep = guess_fitsep(fdt(object)),
  fit = fits(object),
  coef = coefs(object, fit = fit),
  significancevar = "p",
  significance = 0.05
)
```

Arguments

object	SummarizedExperiment
sep	string
fit	character vector
coef	character vector
significancevar	'p' or 'fdr'
significance	fraction : pvalue cutoff

Value

SummarizedExperiment

Examples

```
file <- system.file('extdata/atkin.metabolon.xlsx', package = 'autonomics')
object <- read_metabolon(file, fit = 'limma', coef = 't3-t0')
fdt(object)
fdt(abstract_fit(object))
```

---

add_adjusted_pvalues *Add adjusted pvalues*

Description

Add adjusted pvalues

Usage

```
add_adjusted_pvalues(object, ...)

## S3 method for class 'data.table'
add_adjusted_pvalues(
  object,
  method = "fdr",
  fit = fits(object),
  coefs = autonomics::coefs(object, fit = fit),
  verbose = TRUE,
  ...
)

## S3 method for class 'SummarizedExperiment'
add_adjusted_pvalues(
  object,
  method = "fdr",
  fit = fits(object),
```

```
  coefs = autonomics::coefs(object, fit = fit),
  verbose = TRUE,
  ...
)
```

Arguments

object	SummarizedExperiment or (feature) data.table
...	for s3 dispatch
method	'fdr', 'bonferroni', ... (see 'p.adjust.methods')
fit	'limma', 'lm', 'lme', 'lmer'
coefs	coefficient (string)
verbose	TRUE or FALSE

Value

SummarizedExperiment

Examples

```
file <- system.file('extdata/fukuda20.proteingroups.txt', package = 'autonomics')
object <- read_maxquant_proteingroups(file)
fdt(object) %<>% extract(, 1:2)
object %<>% fit_limma()
object %<>% extract(order(fdt(.)$`p~Adult-X30dpt~limma`), )
 fdt(object)
(fdt(object) %<>% add_adjusted_pvalues('fdr'))
(fdt(object) %<>% add_adjusted_pvalues('fdr'))     # smart enough not to add second column
(fdt(object)  %>% add_adjusted_pvalues('bonferroni'))
```

---

add_assay_means *Add assay means*

Description

Add assay means

Usage

```
add_assay_means(object, assay = assayNames(object)[1], bin = TRUE)
```

Arguments

object	SummarizedExperiment or NULL
assay	string
bin	TRUE or FALSE

Value

SummarizedExperiment

Examples

```
file <- system.file('extdata/fukuda20.proteingroups.txt', package = 'autonomics')
object <- read_maxquant_proteingroups(file)
fdt(object) %<>% extract(, 1:2)
fdt(object)
object %<>% add_assay_means(SummarizedExperiment::assayNames(.))
fdt(object)
```

`add_facetvars` *Add facetvars*

Description

Add facetvars

Usage

```
add_facetvars(
  object,
  fit = fits(object)[1],
  coefs = autonomics::coefs(object, fit = fit)
)
```

Arguments

`object`	SummarizedExperiment
`fit`	string
`coefs`	string vector

Value

SummarizedExperiment

Examples

```
file <- system.file('extdata/atkin.metabolon.xlsx', package = 'autonomics')
object <- read_metabolon(file, fit = 'limma')
object %<>% add_adjusted_pvalues()
fdt(object)
fdt(add_facetvars(object))
```

add_opentargets_by_uniprot *Add opentargets annotations*

Description

Add opentargets annotations

Usage

```
add_opentargets_by_uniprot(
  object,
  cols = c("genesymbol", "genename", "function"),
  verbose = TRUE
)
```

Arguments

object	SummarizedExperiment
cols	character vector
verbose	TRUE or FALSE

Value

SummarizedExperiment

Examples

```
file <- system.file('extdata/billing19.proteingroups.txt', package = 'autonomics')
object <- read_maxquant_proteingroups(file)
object %<>% add_opentargets_by_uniprot()
```

add_psp *Add psp*

Description

Add PhosphoSitePlus literature counts

Usage

```
add_psp(
  object,
  pspfile = file.path(R_user_dir("autonomics", "cache"), "phosphositeplus",
    "Phosphorylation_site_dataset.gz")
)
```

Arguments

object	SummarizedExperiment
pspfile	phosphositeplus file

Details

Go to www.phosphosite.org
Register and Login.
Download Phosphorylation_site_dataset.gz'.
Save into: file.path(R_user_dir('autonomics','cache'),'phosphositeplus')

Value

SummarizedExperiment

Examples

```
fosfile <- system.file('extdata/billing19.phosphosites.txt',  package = 'autonomics')
profile <- system.file('extdata/billing19.proteingroups.txt', package = 'autonomics')
object <- read_maxquant_phosphosites(fosfile = fosfile, profile = profile)
fdt(object)
object %<>% add_psp()
fdt(object)
```

---

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 <- system.file('extdata/atkin.metabolon.xlsx', package = 'autonomics')
object <- read_metabolon(file)
# add_smiles(object[1:10, ]) # seems down
```

`altenrich` *Alternative Enrichment Analysis*

Description

Alternative Enrichment Analysis

Usage

```
altenrich(
  object,
  pathwaydt,
  genevar = "gene",
  genesep = "[ ,;]",
  coef = autonomics::coefs(object)[1],
  fit = fits(object)[1],
  significancevar = "p",
  significance = 0.05,
  effectsize = 0,
  n = 3,
  genes = FALSE,
  verbose = TRUE
)
```

Arguments

`object`	`SummarizedExperiment`
`pathwaydt`	`data.table`, e.g. `read_msigdt`
`genevar`	gene `fvar`
`genesep`	`string` or `NULL`
`coef`	`string` in `coefs(object)`
`fit`	`'limma'`, `'lm'`, `'lme'`, `'lmer'`, `'wilcoxon'`
`significancevar`	'p' or 'fdr'
`significance`	significance cutoff
`effectsize`	effectsize cutoff
`n`	no of detected genes required (for geneset to be examined)
`genes`	whether to record genes
`verbose`	whether to msg

Details

This is an alternative enrichent analysis implementation. It is more modular: uses four times `.enrichment(VERBOSE)?` as backend. But also four times slower than `enrichment`, so not recommended. It is retaind for testing purposes.

This alternative enrichment implementation

See Also

[enrichment()]

`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 <- system.file('extdata/billing19.proteingroups.txt', package = 'autonomics')
object <- read_maxquant_proteingroups(file)
analysis(object)
```

`analyze` *Analyze*

Description

Analyze

Usage

```
analyze(
  object,
  pca = TRUE,
  pls = TRUE,
  fit = "limma",
  formula = ~subgroup,
  drop = varlevels_dont_clash(object, all.vars(formula)),
  codingfun = contr.treatment.explicit,
  contrasts = NULL,
 coefs = contrast_coefs(object, formula = formula, drop = drop, codingfun = codingfun),
  block = NULL,
  weightvar = if ("weights" %in% assayNames(object)) "weights" else NULL,
  plot = pca & !is.null(fit),
  label = "feature_id",
  palette = NULL,
  verbose = TRUE
)
```

Arguments

`object`	SummarizedExperiment
`pca`	TRUE / FALSE: perform pca ?
`pls`	TRUE / FALSE: perform pls ?
`fit`	linmod engine: 'limma', 'lm', 'lme(r)', 'lmer', 'wilcoxon'
`formula`	model formula
`drop`	TRUE / FALSE : drop varname in designmat ?
`codingfun`	factor coding function • contr.treatment: intercept = y0, coefi = yi - y0 • contr.treatment.explicit: intercept = y0, coefi = yi - y0 • code_control: intercept = ymean, coefi = yi - y0 • contr.diff: intercept = y0, coefi = yi - y(i-1) • code_diff: intercept = ymean, coefi = yi - y(i-1) • code_diff_forward: intercept = ymean, coefi = yi - y(i+) • code_deviation: intercept = ymean, coefi = yi - ymean (drop last) • code_deviation_first: intercept = ymean, coefi = yi - ymean (drop first)

- code_helmert: intercept = ymean, coefi = yi - mean(y0:(yi-1))
- code_helmert_forward: intercept = ymean, coefi = yi - mean(y(i+1):yp)

contrasts	model coefficient contrasts of interest: string vector or NULL
coefs	model coefficients of interest: string vector or NULL
block	model blockvar
weightvar	NULL or name of weight matrix in assays(object)
plot	TRUE / FALSE
label	fvar
palette	NULL or colorvector
verbose	TRUE / FALSE: message?

Value

SummarizedExperiment

Examples

```
file <- system.file('extdata/atkin.metabolon.xlsx', package = 'autonomics')
object <- read_metabolon(file)
object %<>% analyze()
```

---

annotate_compounddiscoverer

Read compound discoverer output

Description

Read compound discoverer output

Usage

```
annotate_compounddiscoverer(
  x,
  dir = getwd(),
 files = list.files(path = dir, pattern = ".*masslist.*\\.xlsx$", ignore.case = TRUE,
    full.names = TRUE),
  verbose = TRUE
)
```

Arguments

x	SummarizedExperiment (read_compounddiscoverer)
dir	compound discoverer output directory
files	compound discoverer masslist files
verbose	TRUE or FALSE : message ?

Value

SummarizedExperiment

`annotate_maxquant` *Annotate maxquant*

Description

Annotate maxquant data.table

Usage

```
annotate_maxquant(
  dt,
  uniprothdrs,
  contaminanthdrs,
  maxquanthdrs,
  restapi = FALSE,
  verbose = TRUE
)
```

Arguments

`dt`	`data.table` : output of `read_maxquant_(proteingroups|phosphosites)`
`uniprothdrs`	`data.table` : output of `read_uniprotdt`
`contaminanthdrs`	`data.table` : output of `read_uniprotdt`
`maxquanthdrs`	`data.table` : output of `read_uniprotdt`
`restapi`	`logical(1)` : use uniprot restapi to complete missing annotations ?
`verbose`	`logical(1)` : message ?

Details

Uncollapse, annotate, curate, recollapse, name

Value

`data.table`

Examples

```
# Fukuda 2020: contaminants + maxquanthdrs
#---------------------------------------
        file <- system.file('extdata/fukuda20.proteingroups.txt', package = 'autonomics')
            dt <- .read_maxquant_proteingroups(file)
            dt[, 1:2]
     uniprothdrs <- NULL
 contaminanthdrs <- read_contaminantdt()
    maxquanthdrs <- parse_maxquant_hdrs(dt$`Fasta headers`); dt$`Fasta headers` <- NULL
          dt %<>% annotate_maxquant(uniprothdrs, contaminanthdrs, maxquanthdrs)
          dt[                 , 1:9]
          dt[    reverse== '+', 1:9]
          dt[contaminant== '+', 1:9]

# Billing 2019: uniprothdrs + contaminants + maxquanthdrs
#---------------------------------------------------------
profile <- system.file('extdata/billing19.proteingroups.txt', package = 'autonomics')
fosfile <- system.file('extdata/billing19.phosphosites.txt',  package = 'autonomics')
 upfile <- system.file('extdata/uniprot_hsa_20140515.fasta',  package = 'autonomics')
prodt <- .read_maxquant_proteingroups(profile);         prodt[, 1:2]
fosdt <- .read_maxquant_phosphosites(fosfile, profile); fosdt[, 1:3]
    uniprothdrs <- read_uniprotdt(upfile)
contaminanthdrs <- read_contaminantdt()
   maxquanthdrs <- parse_maxquant_hdrs(prodt$`Fasta headers`)
annotate_maxquant(prodt, uniprothdrs, contaminanthdrs, maxquanthdrs)[, 1:8]
annotate_maxquant(fosdt, uniprothdrs, contaminanthdrs, maxquanthdrs)[, 1:8]
```

---

annotate_uniprot_rest *Annotate uniprot/ensp*

Description

Annotate uniprot/ensp

Usage

```
annotate_uniprot_rest(x, columns = UNIPROTCOLS, verbose = TRUE)
```

Arguments

x	character vector
columns	character vector
verbose	TRUE or FALSE

Value

data.table(dbid, uniprot, reviewed, protein, gene, canonical, isoform, fragment, existence, organism, full)

Examples

```
annotate_uniprot_rest( x = c('P00761', 'Q32MB2') )
annotate_uniprot_rest( x = c('ENSBTAP00000006074', 'ENSP00000377550') )
```

`assert_is_valid_sumexp` *Assert that x is a valid SummarizedExperiment*

Description

Assert that x is a valid SummarizedExperiment

Usage

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

Arguments

x	SummarizedExperiment
.xname	see get_name_in_parent

Value

TRUE or FALSE

Examples

```
# VALID
    file <- system.file('extdata/atkin.metabolon.xlsx', package = 'autonomics')
    x <- read_metabolon(file)
    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 19.

Examples

```
AUTONOMICS_DATASETS
```

`bin` *Bin continuous variable*

Description

Bin continuous variable

Usage

```
bin(object, ...)

## S3 method for class 'logical'
bin(object, ...)

## S3 method for class 'character'
bin(object, ...)

## S3 method for class 'factor'
bin(object, ...)

## S3 method for class 'numeric'
bin(object, probs = c(0, 0.33, 0.66, 1), ...)

## S3 method for class 'SummarizedExperiment'
bin(object, fvar, probs = c(0, 0.33, 0.66, 1), ...)
```

Arguments

`object`	numeric or SummarizedExperiment
`...`	(S3 dispatch)
`probs`	numeric
`fvar`	string or NULL

Value

factor vector

Examples

```
# Numeric vector
    object <- rnorm(10, 5, 1)
    bin(object)
# SummarizedExperiment
    file <- system.file('extdata/fukuda20.proteingroups.txt', package = 'autonomics')
    fdt(object <- read_maxquant_proteingroups(file))
    fdt(bin(object, 'pepcounts'))
```

`biplot` *Biplot*

Description

Biplot

Usage

```
biplot(
  object,
  method = biplot_methods(object)[1],
  by = biplot_by(object, method)[1],
  dims = biplot_dims(object, method, by)[1:2],
  color = if (method %in% DIMREDSUPER) by else "subgroup",
  shape = NULL,
  size = NULL,
  alpha = NULL,
  group = NULL,
  linetype = NULL,
  label = NULL,
  feature_label = "feature_id",
  fixed = list(shape = 15, size = 3),
  nx = 0,
  ny = 0,
  colorpalette = make_svar_palette(object, color),
  alphapalette = make_alpha_palette(object, alpha),
  title = paste0(method, guess_fitsep(fdt(object)), by),
  theme = ggplot2::theme(plot.title = element_text(hjust = 0.5), panel.grid =
    element_blank())
)
```

Arguments

`object`	SummarizedExperiment
`method`	'pca', 'pls', 'lda', 'spls', 'opls', 'sma'
`by`	svar

dims	numeric vector: e.g. 1:2
color	svar
shape	svar
size	svar
alpha	svar
group	svar
linetype	svar
label	svar
feature_label	fvar
fixed	fixed plot aesthetics
nx	number of x features to plot
ny	number of y features to plot
colorpalette	character vector
alphapalette	character vector
title	string
theme	ggplot2::theme output

Value

ggplot object

Examples

```
file <- system.file('extdata/atkin.metabolon.xlsx', package = 'autonomics')
object <- read_metabolon(file)
object %<>% pca(ndim = 4)
object %<>% pls(ndim = 4)
biplot(object)
biplot(object, nx = 1)
biplot(object, dims = 3:4, nx = 1)
biplot(object, method = 'pls')
biplot(object, method = 'pls', dims = 3:4)
biplot(object, method = 'pls', dims = 3:4, group = 'Subject')
```

---

biplot_corrections *Biplot batch corrections*

Description

Biplot batch corrections

Usage

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

Arguments

object	SummarizedExperiment
method	'pca', 'pls', 'lda', or 'sma'
by	svar
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 <- system.file('extdata/atkin.metabolon.xlsx', package = 'autonomics')
object <- read_metabolon(file, pca = TRUE, plot = FALSE)
biplot_corrections(object, color = 'subgroup', covariates = c('Sex', 'Diabetes', 'Subject', 'Time'))
```

---

biplot_covariates *Biplot covariates*

Description

Biplot covariates

Usage

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

Arguments

object	SummarizedExperiment
method	'pca', 'pls', 'lda', or 'sma'
by	svar
block	svar
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 <- system.file('extdata/atkin.metabolon.xlsx', package = 'autonomics')
object <- read_metabolon(file, pca = TRUE)
biplot_covariates(object, covariates = 'subgroup', ndim = 12, dimcols = 3)
biplot_covariates(object, covariates = c('Sex', 'Diabetes', 'Subject', 'Time'))
biplot_covariates(object, covariates = c('Sex', 'Diabetes', 'Subject', 'Time'), ndim = 2)
biplot_covariates(object, covariates = c('subgroup'), dimcols = 3)
```

block2lme *Put block in lme-compatible format*

Description

Put block in lme-compatible format

Usage

```
block2lme(block, ...)

## S3 method for class 'list'
block2lme(block, verbose = TRUE, ...)

## S3 method for class 'formula'
block2lme(block, verbose = TRUE, ...)

## S3 method for class 'character'
block2lme(block, verbose = TRUE, ...)

formula2lmer(formula, block)

formula2lm(formula, block)

block_vars(formula)
```

Arguments

block	block: charactervector or formula
...	required for s3 dispatch
verbose	TRUE or FALSE
formula	formula

Examples

```
# lme: ensure lme-compatiblae block specification
    block2lme( block = list(subject = ~1, batch = ~1))
    block2lme( block =   ~1|subject)
    block2lme( block =   c('subject',    'batch'))

# lm: integrate block into formula as random effect
    formula2lm(   formula = ~ subgroup,  block = c('subject', 'batch') )

# lmer: integrate block into formula as fixed effect
    formula2lmer( formula = ~ subgroup,  block = c('subject',    'batch') )
    formula2lmer( formula = ~ subgroup         + (1|subject) + (1|batch ) )
```

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(matrixStats)
file <- system.file('extdata/fukuda20.proteingroups.txt', package = 'autonomics')
object <- read_maxquant_proteingroups(file)
fdt(object)$housekeeping <- FALSE
fdt(object)$housekeeping[order(rowVars(values(object)))[1:5]] <- TRUE
values(object)[, object$subgroup=='Adult'] %<>% magrittr::add(5)
plot_sample_densities(object)
plot_sample_densities(center(object))
plot_sample_densities(center(object, housekeeping))
```

code *Contrast Code Factor*

Description

Contrast Code Factor for General Linear Model

Usage

```
code(object, ...)

## S3 method for class 'factor'
code(object, codingfun, verbose = TRUE, ...)

## S3 method for class 'data.table'
code(object, codingfun, vars = names(object), verbose = TRUE, ...)

contr.treatment.explicit(n)

code_control(n)

contr.diff(n)

code_diff(n)

code_diff_forward(n)

code_deviation(n)

code_deviation_first(n)

code_helmert(n)

code_helmert_forward(n)
```

Arguments

object	factor vector
...	used for s3 dispatch
codingfun	factor coding function

- contr.treatment: intercept = y0, coefi = yi - y0
- contr.treatment.explicit: intercept = y0, coefi = yi - y0
- code_control: intercept = ymean, coefi = yi - y0
- contr.diff: intercept = y0, coefi = yi - y(i-1)
- code_diff: intercept = ymean, coefi = yi - y(i-1)

- code_diff_forward: intercept = ymean, coefi = yi - y(i+)
- code_deviation: intercept = ymean, coefi = yi - ymean (drop last)
- code_deviation_first: intercept = ymean, coefi = yi - ymean (drop first)
- code_helmert: intercept = ymean, coefi = yi - mean(y0:(yi-1))
- code_helmert_forward: intercept = ymean, coefi = yi - mean(y(i+1):yp)

verbose	TRUE or FALSE
vars	svars
n	character vector

Details

A General Linear Model contains:
* An Intercept Coefficient: expressing some form of sample average
* For each numeric variable: a slope coefficient
* For each k-leveled factor: (k-1) Contrast Coefficients.
The interpretation of (intercept and contrast) coefficients depends on the contrast coding function used. Several contrast coding functions are available in 'stats' and 'codingMatrices' But their (function and coefficient) namings are a bit confusing and unsystematic. Instead, the functions below offer an intuitive interface (to the otherwise powerful stats/codingMatrices packages). The names of these functions reflect the contrast coding used (treatment, backward, sum, or helmert contrasts). They also reflect the intercept interpretation (either first factor's first level or grand mean). They all produce intuitive coefficient names (e.g. 't1-t0' rather than just 't1'). They all have unit scaling (a coefficient of 1 means a backward of 1).

Value

(explicitly coded) factor vector

Examples

```
# Coding functions
    x <- factor(paste0('t', 0:3))
    xlevels <- levels(x)
    contr.treatment(         xlevels)
    contr.treatment.explicit(xlevels)
    contr.diff(              xlevels)
    code_control(            xlevels)
    code_diff(               xlevels)
    code_diff_forward(       xlevels)
    code_deviation(          xlevels)
    code_deviation_first(    xlevels)
    code_helmert(            xlevels)
    code_helmert_forward(    xlevels)

# Code
    x %<>% code(contr.treatment)
    x %<>% code(contr.treatment.explicit)
    x %<>% code(contr.diff)
    x %<>% code(code_control)
```

```
    x %<>% code(code_diff)
    x %<>% code(code_diff_forward)
    x %<>% code(code_deviation)
    x %<>% code(code_deviation_first)
    x %<>% code(code_helmert)
    x %<>% code(code_helmert_forward)

# Model
    file <- system.file('extdata/atkin.metabolon.xlsx', package = 'autonomics')
    object <- read_metabolon(file)
    object %<>% fit_limma(codingfun = contr.treatment) # default
    object %<>% fit_limma(codingfun = contr.treatment.explicit)
    object %<>% fit_limma(codingfun = contr.diff)
    object %<>% fit_limma(codingfun = code_control)
    object %<>% fit_limma(codingfun = code_diff)
    object %<>% fit_limma(codingfun = code_diff_forward)
    object %<>% fit_limma(codingfun = code_deviation)
    object %<>% fit_limma(codingfun = code_deviation_first)
    object %<>% fit_limma(codingfun = code_helmert)
    object %<>% fit_limma(codingfun = code_helmert_forward)
```

`coefs` *Get coefs*

Description

Get coefs

Usage

```
coefs(object, ...)

## S3 method for class 'factor'
coefs(object, intercept = FALSE, ...)

## S3 method for class 'data.table'
coefs(object, fit = fits(object), intercept = FALSE, ...)

## S3 method for class 'SummarizedExperiment'
coefs(object, fit = fits(object), intercept = FALSE, ...)
```

Arguments

`object`	factor, data.table, SummarizedExperiment
`...`	required for s3 dispatch
`intercept`	TRUE or FALSE : whether to include the intercept
`fit`	'limma', 'lm', 'lme', 'lmer', 'wilcoxon'

Value

character vector

Examples

```
# Factor
    x <- factor(c('A', 'B', 'C'))
    coefs(x)
    coefs(code(x, contr.treatment.explicit))
    coefs(code(x, code_control))

# SummarizedExperiment
    file <- system.file('extdata/atkin.metabolon.xlsx', package = 'autonomics')
    object <- read_metabolon(file, fit = 'limma')
    coefs(object)
    coefs(object, intercept = TRUE)
```

---

collapsed_entrezg_to_symbol

Collapsed entrezg to genesymbol

Description

Collapsed entrezg to genesymbol

Usage

```
collapsed_entrezg_to_symbol(x, sep, orgdb)
```

Arguments

x	charactervector
sep	string
orgdb	OrgDb

Value

character vector

Examples

```
if (requireNamespace('org.Hs.eg.db', quiet = TRUE)){
    x <- c('7448/3818/727', '5034/9601/64374')
    orgdb <- org.Hs.eg.db::org.Hs.eg.db
    collapsed_entrezg_to_symbol(x, sep = '/', orgdb = orgdb)
}
```

COMPOUNDDISCOVERER_PATTERNS *compound discoverer quantity patterns*

Description

compound discoverer quantity patterns

Usage

```
COMPOUNDDISCOVERER_PATTERNS
```

Format

An object of class `character` of length 2.

Examples

```
COMPOUNDDISCOVERER_PATTERNS
```

contrast_coefs *Get model coefs*

Description

Get model coefs

Usage

```
contrast_coefs(
  object,
  formula = default_formula(object),
  drop = varlevels_dont_clash(object, all.vars(formula)),
  codingfun = contr.treatment.explicit,
 design = create_design(object, formula = formula, drop = drop, codingfun = codingfun,
    verbose = FALSE)
)

model_coefs(
  object,
  formula = default_formula(object),
  drop = varlevels_dont_clash(object, all.vars(formula)),
  codingfun = contr.treatment.explicit,
 design = create_design(object, formula = formula, drop = drop, codingfun = codingfun,
    verbose = FALSE)
)
```

Arguments

object	SummarizedExperiment
formula	formula
drop	TRUE or FALSE
codingfun	coding function (e.g. contr.treatment)
design	design matrix

Value

SummarizedExperiment

Examples

```
file <- system.file('extdata/atkin.metabolon.xlsx', package = 'autonomics')
object <- read_metabolon(file)
object %<>% fit_limma()
model_coefs(object)
contrast_coefs(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 <- system.file('extdata/atkin.metabolon.xlsx', package = 'autonomics')
object <- read_metabolon(file)
object$subgroup <- paste0(object$Diabetes, '.', object$Time)
subgroup_matrix(object, subgroupvar = 'subgroup')
contrast_subgroup_cols(object, subgroupvar = 'subgroup')
contrast_subgroup_rows(object, subgroupvar = 'subgroup')
```

---

counts *Get/Set counts*

Description

Get / Set counts matrix

Usage

```
counts(object)

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

counts(object) <- value

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

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

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

Arguments

object	SummarizedExperiment
value	count matrix (features x samples)

Value

count matrix (get) or updated object (set)

Examples

```
file <- system.file('extdata/billing19.rnacounts.txt', package = 'autonomics')
object <- read_rnaseq_counts(file)
counts(object)[1:3, 1:3]
counts(object) <- values(object)
```

`counts2cpm` *Convert between counts and cpm/tpm*

Description

Convert between counts and cpm/tpm

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 <- system.file('extdata/billing19.rnacounts.txt', package = 'autonomics')
object <- read_rnaseq_counts(file)
libsize <- scaledlibsizes(counts(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 <- system.file('extdata/billing19.rnacounts.txt', package = 'autonomics')
object <- read_rnaseq_counts(file)
counts(object)[1:3, 1:3]
counts2tpm(counts(object), genesize = 1)[1:3, 1:3]
```

---

count_in *Count/Collapse in/outside intersection*

Description

Count/Collapse in/outside intersection

Usage

```
count_in(x, ...)

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

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

## S3 method for class 'list'
count_in(x, y, ...)

collapse_in(x, ...)

## S3 method for class 'character'
collapse_in(x, y, sep, ...)

## S3 method for class 'factor'
collapse_in(x, y, sep, ...)

## S3 method for class 'list'
collapse_in(x, y, sep, ...)

count_out(x, ...)

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

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

```
count_out(x, y, ...)

## S3 method for class 'list'
count_out(x, y, ...)
```

Arguments

x	character OR list
...	used for S3 dispatch
y	character
sep	string

Value

number OR numeric

Examples

```
# Sets
   contrast1 <- c('a', 'b', 'c', 'd')
     pathway <- c('c', 'd', 'e', 'f')
   contrast2 <- c('e', 'f', 'g', 'h')

# Count outside
   count_out(contrast1, pathway)
   count_out(list(contrast1 = contrast1, contrast2 = contrast2), pathway)

# Count inside
   count_in(contrast1, pathway)
   count_in(list(contrast1 = contrast1, contrast2 = contrast2), pathway)

# Collapse inside
   collapse_in(contrast1, pathway, sep = ' ')
   collapse_in(list(contrast1 = contrast1, contrast2 = contrast2), pathway, sep = ' ')
```

---

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 <- system.file('extdata/billing19.rnacounts.txt', package = 'autonomics')
object <- read_rnaseq_counts(file)
cpm(object)[1:3, 1:3]
cpm(object) <- values(object)
```

---

create_design *Create design matrix*

Description

Create design matrix for statistical analysis

Usage

```
create_design(object, ...)

## S3 method for class 'SummarizedExperiment'
create_design(
  object,
  formula = default_formula(object),
  drop = varlevels_dont_clash(object, all.vars(formula)),
  codingfun = contr.treatment.explicit,
  verbose = TRUE,
  ...
)

## S3 method for class 'data.table'
create_design(
```

```
  object,
  formula = default_formula(object),
  drop = varlevels_dont_clash(object, all.vars(formula)),
  codingfun = contr.treatment.explicit,
  verbose = TRUE,
  ...
)
```

Arguments

object	SummarizedExperiment or data.frame
...	required to s3ify
formula	formula with svars
drop	whether to drop predictor names
codingfun	factor coding function
	• contr.treatment: intercept = y0, coefi = yi - y0
	• contr.treatment.explicit: intercept = y0, coefi = yi - y0
	• code_control: intercept = ymean, coefi = yi - y0
	• contr.diff: intercept = y0, coefi = yi - y(i-1)
	• code_diff: intercept = ymean, coefi = yi - y(i-1)
	• code_diff_forward: intercept = ymean, coefi = yi - y(i+)
	• code_deviation: intercept = ymean, coefi = yi - ymean (drop last)
	• code_deviation_first: intercept = ymean, coefi = yi - ymean (drop first)
	• code_helmert: intercept = ymean, coefi = yi - mean(y0:(yi-1))
	• code_helmert_forward: intercept = ymean, coefi = yi - mean(y(i+1):yp)
verbose	whether to message

Value

design matrix

Examples

```
file <- system.file('extdata/atkin.metabolon.xlsx', package = 'autonomics')
object <- read_metabolon(file)
unique(create_design(object))
unique(create_design(object, ~ Time))
unique(create_design(object, ~ Time, codingfun = contr.treatment.explicit))
unique(create_design(object, ~ Time, codingfun = contr.diff))
unique(create_design(object, ~ Time + Diabetes))
unique(create_design(object, ~ Time / Diabetes))
unique(create_design(object, ~ Time * Diabetes))
```

DATADIR *Download autonomics example data*

Description

Download autonomics example data

Usage

```
DATADIR

download_data(
  filename = NULL,
  localdir = file.path(DATADIR, split_extract_fixed(filename, ".", 1)),
  verbose = TRUE,
  force = FALSE
)
```

Arguments

`filename` file name

'atkin.somascan.adat'	Halama, 2018	effects of hypoglycemia
'atkin.metabolon.xlsx'		
'billing16.bam.zip'	Billing, 2016	stemcell comparison
'billing16.rnacounts.txt'		
'billing16.somascan.adat'		
'billing16.proteingroups.txt'		
'billing19.rnacounts.txt'	Billing, 2016	stemcell differentiation
'billing19.proteingroups.txt'		
'billing19.phosphosites.txt'		
'ddglucose.proteingroups.txt'	Omics Module	glycolysis inhibitor
'fukuda20.proteingroups.txt'	Fukuda, 2020	zebrafish development
'halama18.metabolon.xlsx'	Halama, 2018	glutaminase inhibitor

`localdir` local dir to save file to

`verbose` TRUE / FALSE

`force` TRUE / FALSE

Format

An object of class `character` of length 1.

Value

local file path

Examples

```
# Show available datasets
    download_data()

# atkin 2018 - hypoglycemia - pubmed 30525282
    # download_data('atkin.somascan.adat')            # somascan  intensities
    # download_data('atkin.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
```

`default_geom` *Default geom*

Description

Default geom

Usage

```
default_geom(object, x, block = NULL)
```

Arguments

`object`	SummarizedExperiment
`x`	svar
`block`	svar or NULL

Value

character vector

Examples

```
file <- system.file('extdata/atkin.metabolon.xlsx', package = 'autonomics')
object <- read_metabolon(file)
object$Age <- runif(min = 20, max = 60, n = ncol(object))
svars(object)
default_geom(object, x = 'Age')
default_geom(object, x = c('Age', 'Diabetes'))
default_geom(object, x = c('Age', 'Diabetes'), block = 'Subject')
```

---

default_sfile *Default sfile*

Description

Default sfile

Usage

```
default_sfile(file)
```

Arguments

file	data file

Value

sample file

Examples

```
file <- system.file('extdata/billing19.proteingroups.txt', package = 'autonomics')
default_sfile(file)
```

---

default_subgroupvar *Create default formula*

Description

Create default formula

Usage

```
default_subgroupvar(object)

default_formula(object)
```

Arguments

object	SummarizedExperiment

Value

formula

Examples

```
# Abundances
    file <- system.file('extdata/atkin.metabolon.xlsx', package = 'autonomics')
    object <- read_metabolon(file)
    default_formula(object)
    file <- download_data('billing16.proteingroups.txt')
    object <- read_maxquant_proteingroups(file)
    default_formula(object)
```

---

demultiplex *Demultiplex snames*

Description

Demultiplex maxquant samplenames

Usage

```
demultiplex(x, verbose = FALSE)
```

Arguments

x	character vector
verbose	TRUE or FALSE

Details

WT(L).KD(H).R1{H/L} -> KD_WT.R1 WT(1).KD(2).R1{1} -> WT.R1 WT.R1 -> WT.R1

Value

character

Examples

```
# uniplexed / intensity / ratio
   demultiplex(c('KD.R1','OE.R1'))
   demultiplex(c('WT(L).KD(M).OE(H).R1{M}',  'WT(L).KD(M).OE(H).R1{H}'))
   demultiplex(c('WT(L).KD(M).OE(H).R1{M/L}','WT(L).KD(M).OE(H).R1{H/L}'))
# run / replicate
   demultiplex(c('WT(L).OE(H).R1{L}',    'WT(L).OE(H).R1{H}'))     # run
   demultiplex(c('WT.R1(L).OE.R1(H){L}', 'WT.R1(L).OE.R1(H){H}'))  # repl
# label / index
   demultiplex(c('WT(L).OE(H).R1{L}',    'WT(L).OE(H).R1{H}'))     # label
   demultiplex(c('WT(1).OE(2).R1{1}',    'WT(1).OE(2).R1{2}'))     # index
# with unused channels
   demultiplex('WT(1).KD(2).OE(3).R1{6}')
```

---

dequantify *Dequantify maxquant snames*

Description

Drop quantity ('Reporter intensity').
Encode {channel} as suffix.

Usage

```
dequantify(x, quantity = guess_maxquant_quantity(x), verbose = FALSE)
```

Arguments

x	character
quantity	'ratio', 'normalizedratio', 'LFQ intensity', 'intensity', 'labeledintensity' 'reporterintensity', 'correctedreporterintensit
verbose	TRUE or FALSE

Details

```
           Ratio H/L WT(L).KD(H).R1  ->  WT(L).KD(H).R1{H/L}              LFQ intensity WT.R1  ->  WT.R1
Reporter intensity 0 WT(126).KD(127).R1  ->  WT(1).KD(2).R1{1}
```

Value

character

Examples

```
dequantify(c('Ratio H/L WT(L).KD(M).OE(H).R1',            # Ratios
             'Ratio M/L WT(L).KD(M).OE(H).R1'))
dequantify(c('Ratio H/L normalized WT(L).KD(M).OE(H).R1',  # Norm. Ratios
             'Ratio M/L normalized WT(L).KD(M).OE(H).R1'))
dequantify(c('LFQ intensity WT.R1',                        # LFQ intensity
             'LFQ intensity KD.R1'))
dequantify(c('Reporter intensity 1 WT(126).KD(127).R1',    # Rep.intensities
             'Reporter intensity 2 WT(126).KD(127).R1'))
```

---

dequantify_compounddiscoverer

dequantify_compounddiscoverer compound discoverer snames

Description

Drop quantity.

Usage

```
dequantify_compounddiscoverer(
  x,
  quantity = guess_compounddiscoverer_quantity(x),
  verbose = FALSE
)
```

Arguments

x	character
quantity	'area', 'normalizedarea'
verbose	TRUE or FALSE

Details

Norm. Area: 20230908_F143_HILICNEG.raw (F11) -> 20230908_F143_HILICNEG.raw (F11)
Area: 20230908_F143_HILICNEG.raw (F11) -> 20230908_F143_HILICNEG.raw (F11)

Value

character

Examples

```
dequantify_compounddiscoverer("Norm. Area: 20230908_F143_HILICNEG.raw (F11)") # Norm. Area
dequantify_compounddiscoverer("Area: 20230908_F143_HILICNEG.raw (F11)")       # Area
```

DIMREDUN *Dimension Reduction Methods*

Description

Dimension Reduction Methods

Usage

```
DIMREDUN

DIMREDSUPER

DIMREDENGINES
```

Format

An object of class `character` of length 2.

An object of class `character` of length 4.

An object of class `character` of length 6.

Details

- `DIMREDUN: c('pca', 'sma')`
- `DIMREDSUPER: c('lda', 'pls', 'opls', 'spls')`
- `DIMREDENGINES: c('pca', 'sma', 'lda', 'pls', 'opls', 'spls')`

download_gtf *Download GTF file*

Description

Download GTF file with feature annotations

Usage

```
download_gtf(
  organism,
  release = 100,
  gtffile = sprintf("%s/gtf/%s", R_user_dir("autonomics", "cache"),
    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)
```

---

download_mcclain21 *Download mcclain21 data*

Description

Download mcclain21 data

Usage

```
download_mcclain21(
  counts_or_samples = "counts",
  localdir = file.path(DATADIR, "mcclain21"),
  force = FALSE
)
```

Arguments

counts_or_samples	'counts' or 'samples'
localdir	dirname
force	TRUE or FALSE

Details

Mc clain 2021: COVID19 transcriptomics:

Examples

```
download_mcclain21('counts')
download_mcclain21('samples')
```

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')
```

enrichment *Enrichment analysis*

Description

Are selected genes enriched in pathway?

Usage

```
enrichment(
  object,
  pathwaydt,
  fit = fits(object)[1],
  coef = coefs(object, fit = fit)[1],
  var = abstractvar(object, fit = fit, coef = coef),
```

```
  levels = fdt(object)[[var]] %>% base::levels() %>% extract(-1),
  genevar = "gene",
  genesep = "[ ,;]",
  n = 3,
  verbose = TRUE,
  genes = FALSE
)
```

Arguments

object	SummarizedExperiment
pathwaydt	pathway data.table
fit	string
coef	string
var	selection fvar
levels	selection levels
genevar	gene fvar
genesep	gene separator (string)
n	number
verbose	whether to msg
genes	whether to report genes

Details

Four enrichment analyses per geneset using the Fisher Exact Test (see four pvalues). Results are returned in a data.table

in	: genes in pathway
in.det	: detected genes in pathway
in.sel	: up/downregulated genes in pathway
in.up(.genes)	: upregulated genes in pathway
in.down(.genes)	: downregulated genes in pathway
out	: genes outside pathway
det	: detected genes (in + out)
sel	: up/downregulated genes (in + out)
up	: upregulated genes (in + out)
down	: downregulated genes (in + out)
p.coef.upDET	: prob to randomly select this many (or more) upregulated genes (among detected genes)
p.coef.downDET	: prob to randomly select this many (or more) downregulated genes (among detected genes)
p.coef.selDET	: prob to randomly select this many (or more) up OR downregulated genes (among detected genes)
p.coef.selGEN	: prob to randomly select this many (or more) up OR downregulated genes (among genome genes)
p.detGEN	: prob to randomly select this many (or more) detected genes (among genome genes)

Examples

```
# Read
    pathwaydt <- read_msigdt(collections = 'C5:GO:BP')
    file <- system.file('extdata/atkin.somascan.adat', package = 'autonomics')
    object <- read_somascan(file, fit = 'limma', coefs = 't1-t0')
    fvars(object) %<>% gsub('EntrezGeneSymbol', 'gene', .)
    object %<>% abstract_fit()
    varlevels <- c('flat', 'down', 'up')
  enrichdt1 <- enrichment(object, pathwaydt, var = 't1-t0~limma')              # 2:n factor
  enrichdt2 <- enrichment(object, pathwaydt, var = 't1-t0~limma', levels = varlevels)  # 1:n factor
   enrichdt3 <-  altenrich(object, pathwaydt)               # alternative implementation
    cols <- intersect(names(enrichdt1), names(enrichdt3))
   all(enrichdt1[, cols, with = FALSE]  ==  enrichdt3[, cols, with = FALSE])   # identical
```

---

ens2org *taxon/ens to organism*

Description

taxon/ens to organism

Usage

```
ens2org(x)

taxon2org(x)
```

Arguments

x	character vector

Value

character vector

Examples

```
taxon2org( x = c('9606', '9913') )
  ens2org( x = c('ENSP00000377550', 'ENSBTAP00000038329') )
```

entrezg_to_symbol *Entrezg to genesymbol*

Description

Entrezg to genesymbol

Usage

```
entrezg_to_symbol(x, orgdb)
```

Arguments

x	charactervector
orgdb	OrgDb

Value

character vector

Examples

```
if (requireNamespace('org.Hs.eg.db', quiet = TRUE)){
    orgdb <- org.Hs.eg.db::org.Hs.eg.db
    entrezg_to_symbol(x = c('7448', '3818', '727'), orgdb)
}
```

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

Description

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

Usage

```
extract_rectangle(x, ...)

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

```
  sheet = 1,
  ...
)

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

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

Arguments

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

Value

matrix

Examples

```
# FROM FILE: extract_rectangle.character
#=======================================
   x <- system.file('extdata/atkin.metabolon.xlsx', package = 'autonomics')
   extract_rectangle(x, rows = 11:30, cols = 15:81, sheet = 2)[ 1:3, 1:3 ]  # exprs
   extract_rectangle(x, rows = 11:30, cols = 2,     sheet = 2)[ 1:3,     ]  # fids
   extract_rectangle(x, rows = 4,     cols = 15:81, sheet = 2)[    , 1:3 ]  # sids
   extract_rectangle(x, rows = 10:30, cols = 1:14,  sheet = 2)[ 1:3, 1:3 ]  # fdt
```

```
  extract_rectangle(x, rows = 1:10,  cols = 14:81, sheet = 2, transpose = TRUE)[1:3, 1:3] # sdt

# FROM MATRIX: extract_rectangle.matrix
#=====================================
   x <- system.file('extdata/atkin.metabolon.xlsx', package = 'autonomics')
   x %<>% extract_rectangle(sheet = 2)
   extract_rectangle(x, rows = 11:30,  cols = 15:81, sheet = 2)[ 1:3, 1:3 ]  # exprs
   extract_rectangle(x, rows = 11:30,  cols = 2,     sheet = 2)[ 1:3,     ]  # fids
   extract_rectangle(x, rows = 4,      cols = 15:81, sheet = 2)[    , 1:3 ]  # sids
   extract_rectangle(x, rows = 10:30,  cols = 1:14,  sheet = 2)[ 1:3, 1:3 ]  # fdt
  extract_rectangle(x, rows = 1:10,  cols = 14:81, sheet = 2, transpose = TRUE)[1:3, 1:3] # sdt
```

`fcluster` *Cluster features*

Description

Cluster features

Usage

```
fcluster(
  object,
  distmat = NULL,
  method = "cmeans",
  k = 2:10,
  verbose = TRUE,
  plot = TRUE,
  label = if ("gene" %in% fvars(object)) "gene" else "feature_id",
  alpha = 1,
  nrow = if (length(method) > 1) length(method) else NULL,
  ncol = NULL
)
```

Arguments

`object`	SummarizedExperiment
`distmat`	distance matrix
`method`	'cmeans'
`k`	number of clusters
`verbose`	TRUE or FALSE
`plot`	TRUE or FALSE
`label`	fvar
`alpha`	fraction
`nrow`	number
`ncol`	number

Value

SummarizedExperiment

SummarizedExperiment

Examples

```
object <- twofactor_sumexp()
distmat <- fdist(object)
fcluster(object)                                          # membership-based colors
fcluster(object, distmat)                                 # silhouette-based colors
fcluster(object, distmat, method = c('cmeans', 'hclust', 'pamk'))  # more methods
```

---

fdata *Get/Set sample/feature data*

Description

Get/Set sample/feature data

Usage

```
fdata(object)

sdata(object)

fdt(object)

sdt(object)

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

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

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

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

fdata(object) <- value

sdata(object) <- value

fdt(object) <- value
```

```
sdt(object) <- value

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

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

Arguments

object	SummarizedExperiment
value	data.frame/data.table

Value

data.frame/data.table (get) or updated object (set)

Examples

```
# Read data
    file <- system.file('extdata/billing19.proteingroups.txt', package = 'autonomics')
    object <- read_maxquant_proteingroups(file)
# sdt/fdt
    sdt(object)[1:3, ]
    fdt(object)[1:3, ]
    sdt(object) %<>% cbind(b=1)
    fdt(object) %<>% cbind(b=1)
    sdt(object)
    fdt(object)
# sdata/fdata
    sdata(object)[1:3, ]
    fdata(object)[1:3, ]
    sdata(object) %<>% cbind(a=1)
    fdata(object) %<>% cbind(a=1)
    sdata(object)[1:3, ]
    fdata(object)[1:3, ]
```

fdr2p *fdr to p*

Description

fdr to p

Usage

```
fdr2p(fdr)
```

Arguments

fdr	fdr values

Examples

```
# Read/Fit
   file <- system.file('extdata/atkin.metabolon.xlsx', package = 'autonomics')
   object <- read_metabolon(file)
   object %<>% fit_limma()
   pcol <- pvar(fdt(object), fit = 'limma', coef = 't3-t0')
   object %<>% extract(order(fdt(.)[[pcol]]), )
   object %<>% extract(1:10, )
   fdt(object) %<>% extract(, 1)
   object %<>% fit_limma()
# fdr2p
   fdt(object)[[pcol]]
   fdt(object)[[pcol]] %>% p.adjust(method = 'fdr')
   fdt(object)[[pcol]] %>% p.adjust(method = 'fdr') %>% fdr2p()
```

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",
  assay = assayNames(object)[1],
  comparator = if (contains_ratios(object)) "!=" else ">",
  lod = 0,
```

```
  nsample = 2,
  nsubgroup = 1,
  verbose = TRUE
)
```

Arguments

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

Value

Filtered SummarizedExperiment

Examples

```
file <- system.file('extdata/atkin.metabolon.xlsx', package = 'autonomics')
object <- read_metabolon(file)
object %<>% filter_exprs_replicated_in_some_subgroup()
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 = TRUE)
```

Arguments

object	SummarizedExperiment
condition	filter condition
verbose	logical

Value

filtered eSet

Examples

```
file <- system.file('extdata/atkin.metabolon.xlsx', package = 'autonomics')
object <- read_metabolon(file)
filter_features(object, SUPER_PATHWAY == 'Lipid')
```

`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

```
file <- system.file('extdata/billing19.rnacounts.txt', package = 'autonomics')
object <- read_rnaseq_counts(file, plot = FALSE)
object %<>% filter_medoid(by = 'subgroup', verbose=TRUE)
```

filter_samples *Filter samples on condition*

Description

Filter samples on condition

Usage

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

Arguments

object	SummarizedExperiment
condition	filter condition
verbose	TRUE/FALSE
record	TRUE/FALSE

Value

filtered SummarizedExperiment

Examples

```
file <- system.file('extdata/atkin.metabolon.xlsx', package = 'autonomics')
object <- read_metabolon(file)
filter_samples(object, subgroup != 't0', verbose = TRUE)
```

fitcoefs *fitcoefs*

Description

fitcoefs

Usage

```
fitcoefs(object)
```

Arguments

object	SummarizedExperiment

Value

string vector

Examples

```
file <- system.file('extdata/atkin.metabolon.xlsx', package = 'autonomics')
object <- read_metabolon(file)
fitcoefs(object)
fitcoefs(fit_limma(object))
```

`fits` *Get fit models*

Description

Get fit models

Usage

```
fits(object, ...)

## S3 method for class 'data.table'
fits(object, ...)

## S3 method for class 'SummarizedExperiment'
fits(object, ...)
```

Arguments

`object`	SummarizedExperiment or data.table
`...`	S3 dispatch

Value

character vector

Examples

```
file <- system.file('extdata/atkin.metabolon.xlsx', package = 'autonomics')
object <- read_metabolon(file, fit = 'limma')
fits(object)
```

FITSEP *Fit results separator*

Description

Fit results separator

Usage

```
FITSEP

PPATTERN
```

Format

An object of class `character` of length 1.

An object of class `character` of length 1.

Examples

```
FITSEP
```

fit_linmod *Fit General Linear Model*

Description

Fit General Linear Model

Usage

```
fit_linmod(
  object,
  formula = as.formula("~ subgroup"),
  engine = "limma",
  drop = varlevels_dont_clash(object, all.vars(formula)),
  codingfun = contr.treatment.explicit,
 design = create_design(object, formula = formula, drop = drop, codingfun = codingfun,
    verbose = FALSE),
  contrasts = NULL,
  coefs = if (is.null(contrasts)) model_coefs(design = design) else NULL,
  block = NULL,
  weightvar = if ("weights" %in% assayNames(object)) "weights" else NULL,
  sep = FITSEP,
  suffix = paste0(sep, engine),
```

```
  verbose = TRUE,
  outdir = NULL,
  writefun = "write_xl",
  volcano = FALSE,
  volcanoargs = list(),
  exprs = FALSE,
  exprargs = list(),
  ...
)

fit_limma(
  object,
  formula = as.formula("~ subgroup"),
  drop = varlevels_dont_clash(object, all.vars(formula)),
  codingfun = contr.treatment.explicit,
 design = create_design(object, formula = formula, drop = drop, codingfun = codingfun),
  contrasts = NULL,
  block = NULL,
  weightvar = if ("weights" %in% assayNames(object)) "weights" else NULL,
  sep = FITSEP,
  suffix = paste0(sep, "limma"),
  verbose = TRUE
)

.fit_limma(
  object,
  formula = as.formula("~ subgroup"),
  drop = varlevels_dont_clash(object, all.vars(formula)),
  codingfun = contr.treatment.explicit,
 design = create_design(object, formula = formula, drop = drop, codingfun = codingfun),
  contrasts = NULL,
  block = NULL,
  weightvar = if ("weights" %in% assayNames(object)) "weights" else NULL,
  sep = FITSEP,
  suffix = paste0(sep, "limma"),
  verbose = TRUE
)

fit_lm(
  object,
  formula = as.formula("~ subgroup"),
  drop = varlevels_dont_clash(object, all.vars(formula)),
  codingfun = contr.treatment.explicit,
  design = NULL,
  block = NULL,
  weightvar = if ("weights" %in% assayNames(object)) "weights" else NULL,
  sep = FITSEP,
  suffix = paste0(sep, "lm"),
```

```
  contrasts = NULL,
  verbose = TRUE
)

fit_lme(
  object,
  formula = as.formula("~ subgroup"),
  drop = varlevels_dont_clash(object, all.vars(formula)),
  codingfun = contr.treatment.explicit,
  design = NULL,
  block = NULL,
  weightvar = if ("weights" %in% assayNames(object)) "weights" else NULL,
  opt = "optim",
  sep = FITSEP,
  suffix = paste0(sep, "lme"),
  contrasts = NULL,
  verbose = TRUE
)

fit_lmer(
  object,
  formula = as.formula("~ subgroup"),
  drop = varlevels_dont_clash(object, all.vars(formula)),
  codingfun = contr.treatment.explicit,
  design = NULL,
  block = NULL,
  weightvar = if ("weights" %in% assayNames(object)) "weights" else NULL,
  sep = FITSEP,
  suffix = paste0(sep, "lmer"),
  contrasts = NULL,
  verbose = TRUE
)

fit_wilcoxon(
  object,
  formula = as.formula("~ subgroup"),
  drop = NULL,
  codingfun = contr.treatment.explicit,
  design = NULL,
  contrasts = NULL,
  block = NULL,
  weightvar = NULL,
  sep = FITSEP,
  suffix = paste0(sep, "wilcoxon"),
  verbose = TRUE
)
```

Arguments

object	SummarizedExperiment
formula	model formula
engine	'limma', 'lm', 'lme', 'lmer', or 'wilcoxon'
drop	TRUE or FALSE
codingfun	factor coding function • contr.treatment: intercept = y0, coefi = yi - y0 • contr.treatment.explicit: intercept = y0, coefi = yi - y0 • code_control: intercept = ymean, coefi = yi - y0 • contr.diff: intercept = y0, coefi = yi - y(i-1) • code_diff: intercept = ymean, coefi = yi - y(i-1) • code_diff_forward: intercept = ymean, coefi = yi - y(i+) • code_deviation: intercept = ymean, coefi = yi - ymean (drop last) • code_deviation_first: intercept = ymean, coefi = yi - ymean (drop first) • code_helmert: intercept = ymean, coefi = yi - mean(y0:(yi-1)) • code_helmert_forward: intercept = ymean, coefi = yi - mean(y(i+1):yp)
design	design matrix
contrasts	NULL or character vector: coefficient contrasts to test
coefs	NULL or character vector: model coefs to test
block	block svar (or NULL)
weightvar	NULL or name of weight matrix in assays(object)
sep	string: pvar separator ("~" in "p~t2~limma")
suffix	string: pvar suffix ("limma" in "p~t2~limma")
verbose	whether to msg
outdir	NULL or dir
writefun	'write_xl' or 'write_ods'
volcano	TRUE or FALSE
volcanoargs	list: volcano args
exprs	TRUE or FALSE
exprargs	list: expr args
...	passed to fit_(limma|lm|lme|lmer) functions
opt	lme options

Value

Updated SummarizedExperiment

Examples

```
# Standard usage
  file <- system.file('extdata/atkin.metabolon.xlsx', package = 'autonomics')
  object <- read_metabolon(file)
  object %<>% fit_linmod()                                # Default
  object %<>% fit_linmod(  ~subgroup )                    # Custom formula
  object %<>% fit_linmod(  ~subgroup, block = 'Subject')  # Block effect
  summarize_fit(object)

# Alternative engines: argument 'engine' or dedicated function
  fdt(object) %<>% extract(, 'feature_id')
  object %<>% fit_limma(   ~subgroup, block = 'Subject')  # Default engine
  object %<>% fit_lm(      ~subgroup, block = 'Subject')  # Traditional
  object %<>% fit_lme(     ~subgroup, block = 'Subject')  # Powerful random effects
 object %<>% fit_lmer(   ~subgroup, block = 'Subject')  # Yet more powerful random effects
  object %<>% fit_wilcoxon(~subgroup, block = 'Subject')  # Non-parametric
  summarize_fit(object)

# Alternative coding: backward diffs instead of baseline
  fdt(object) %<>% extract(, 'feature_id')
  object %<>% fit_limma(     ~ subgroup, block = 'Subject', codingfun = code_diff)
  object %<>% fit_lme(       ~ subgroup, block = 'Subject', codingfun = code_diff)
  object %<>% fit_lmer(      ~ subgroup, block = 'Subject', codingfun = code_diff)
  summarize_fit(object)

# Posthoc contrasts: limma-only, flexible, but sometimes approximate
  fdt(object) %<>% extract(, 'feature_id')
  object %<>% fit_limma( ~ subgroup, block = 'Subject', codingfun = code_control)
  object %<>% fit_limma( ~ 0 + subgroup, block = 'Subject', contrasts = 't1-t0')
      # flexible, but only approximate
      # stat.ethz.ch/pipermail/bioconductor/2014-February/057682.html

# Custom separator
  fdt(object) %<>% extract(, 'feature_id')
  fdt( fit_limma(object, sep = '.'))
  fdt( fit_limma(object, block = 'Subject', sep = '.') )

# Top-level function also plots and writes
  fit_linmod(object, block = 'Subject', coefs = 't1-t0')
  fit_linmod(object, block = 'Subject', coefs = 't1-t0', volcano = TRUE)
  fit_linmod(object, block = 'Subject', coefs = 't1-t0',   exprs = TRUE)
  fit_linmod(object, block = 'Subject', coefs = 't1-t0', volcano = TRUE, exprs = TRUE)
 fit_linmod(object, block = 'Subject', coefs = 't1-t0', volcano = TRUE, exprs = TRUE, outdir = tempdir())
 fit_linmod(object, block = 'Subject', coefs = 't1-t0', volcano = TRUE, exprs = TRUE, outdir = tempdir())
```

`fix_xlgenes` *Fix excel genes*

Description

Fix excel genes

Usage

```
fix_xlgenes(x)
```

Arguments

x	character

Value

character

Examples

```
x <- c('FAM46B', '15-Sep', '2-Mar', 'MARCHF6')
x
fix_xlgenes(x)
```

---

flevels *Get fvar levels*

Description

Get fvar levels

Usage

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

Arguments

object	SummarizedExperiment
fvar	feature variable

Value

fvar values

Examples

```
file <- system.file('extdata/billing19.proteingroups.txt', package = 'autonomics')
object <- read_maxquant_proteingroups(file)
head(flevels(object, 'feature_id'))
```

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

```
file <- system.file('extdata/billing19.proteingroups.txt', package = 'autonomics')
object <- read_maxquant_proteingroups(file)
fnames(object) %<>% paste0('protein_', .)
object
```

formula2str *formula to string*

Description

formula to string

Usage

```
formula2str(formula)
```

Arguments

formula	formula

Value

string

Examples

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

---

ftype *Feature type*

Description

Feature type

Usage

```
ftype(
  object,
  formula = default_formula(object),
  drop = varlevels_dont_clash(object, all.vars(formula)),
  fit = fits(object)[1],
  codingfun = contr.treatment.explicit
)
```

Arguments

object	SummarizedExperiment
formula	model formula
drop	TRUE or FALSE
fit	'limma', 'lm', 'lme', 'wilcoxon'
codingfun	coding function

Value

SummarizedExperiment

Examples

```
file <- download_data('atkin.metabolon.xlsx')
object <- read_metabolon(file)
object %<>% fit_limma(block = 'Subject') # model_coefs !
object %<>% ftype()          # model_coefs not contrast_coefs !
fdt(object)                  # because intercept is required to recreate predictions
```

fvalues *Get fvalues*

Description

Get fvar values

Usage

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

Arguments

object	SummarizedExperiment
fvar	feature variable

Value

fvar values

Examples

```
file <- system.file('extdata/billing19.proteingroups.txt', package = 'autonomics')
object <- read_maxquant_proteingroups(file)
head(fvalues(object, 'feature_id'))
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

```
file <- system.file('extdata/billing19.proteingroups.txt', package = 'autonomics')
object <- read_maxquant_proteingroups(file)
fvars(object)[1] %<>% paste0('1')
fvars(object)[1]
```

---

genome_to_orgdb *Get corresponding orgdb*

Description

Get corresponding orgdb

Usage

```
genome_to_orgdb(genome)
```

Arguments

genome	'hg38', 'hg19', 'mm10', or 'mm9'

Value

OrgDb

Examples

```
if (requireNamespace('org.Hs.eg.db', quiet = TRUE)){
    class(genome_to_orgdb('hg38'))
}
```

group_by_level *group by level*

Description

group by level

Usage

```
group_by_level(x, ...)

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

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

## S3 method for class 'data.table'
group_by_level(x, var, idvar, ...)
```

Arguments

x	named logical/character/factor
...	S3 dispatch
var	string
idvar	string

Value

unnamed character

Examples

```
t1 <- c( KLF5 = 'up',  F11 = 'up', RIG = 'flat',   ABT1 = 'down')
dt <- data.table( gene = c( 'KL5', 'F11', 'RIG',  'ABT1' ),
                  t1 = c( 'up',  'up',  'flat', 'down' ) )
group_by_level(t1)               #  character
group_by_level(factor(t1))       #     factor
group_by_level(dt, 't1', 'gene')  # data.table
```

guess_compounddiscoverer_quantity *Guess compound discoverer quantity from snames*

Description

Guess compound discoverer quantity from snames

Usage

```
guess_compounddiscoverer_quantity(x)
```

Arguments

x	character vector

Value

string: value from names(COMPOUNDDISCOVERER_PATTERNS)

Examples

```
## Not run:
# file
    file <- system.file('extdata/fukuda20.proteingroups.txt', package = 'autonomics')
    guess_compounddiscoverer_quantity(file)

## End(Not run)

# character vector
    x <- "Area: 20230908_F143_HILICNEG.raw (F11)"
    guess_compounddiscoverer_quantity(x)

    x <- "Norm. Area: 20230908_F143_HILICNEG.raw (F11)"
    guess_compounddiscoverer_quantity(x)
```

guess_fitsep *guess fitsep*

Description

guess fitsep

Usage

```
guess_fitsep(object, ...)

## S3 method for class 'data.table'
guess_fitsep(object, ...)

## S3 method for class 'SummarizedExperiment'
guess_fitsep(object, ...)
```

Arguments

object	data.table or SummarizedExperiment
...	S3 dispatch

Value

string

Examples

```
file <- system.file('extdata/fukuda20.proteingroups.txt', package = 'autonomics')
object <- read_maxquant_proteingroups(file)
object %<>% fit_limma()
guess_fitsep(object)
```

---

guess_maxquant_quantity

Guess maxquant quantity from snames

Description

Guess maxquant quantity from snames

Usage

```
guess_maxquant_quantity(x)
```

Arguments

x	character vector

Value

string: value from names(MAXQUANT_PATTERNS)

Examples

```
# file
    file <- system.file('extdata/fukuda20.proteingroups.txt', package = 'autonomics')
    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)
```

---

guess_sep *Guess separator*

Description

Guess separator

Usage

```
guess_sep(x, ...)

## S3 method for class 'numeric'
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
   guess_sep(c('PERM_NON.R1[H/L]', 'PERM_NON.R2[H/L]'))
   guess_sep(c('WT_untreated_1', 'WT_untreated_2'))
   guess_sep(c('group1', 'group2.R1'))
# SummarizedExperiment
   file <- system.file('extdata/atkin.metabolon.xlsx', package = 'autonomics')
   object <- read_metabolon(file)
   guess_sep(object)
```

---

has_multiple_levels *Variable has multiple levels?*

Description

Variable has multiple levels?

Usage

```
has_multiple_levels(x, ...)

## S3 method for class 'character'
has_multiple_levels(x, .xname = get_name_in_parent(x), ...)

## S3 method for class 'factor'
has_multiple_levels(x, .xname = get_name_in_parent(x), ...)

## S3 method for class 'numeric'
has_multiple_levels(x, .xname = get_name_in_parent(x), ...)

## S3 method for class 'data.table'
has_multiple_levels(
  x,
  y,
```

```
  .xname = get_name_in_parent(x),
  .yname = get_name_in_parent(y),
  ...
)

## S3 method for class 'SummarizedExperiment'
has_multiple_levels(
  x,
  y,
  .xname = get_name_in_parent(x),
  .yname = get_name_in_parent(y),
  ...
)
```

Arguments

x	vector, data.table or SummarizedExperiment
...	required for s3 dispatch
.xname	string
y	string
.yname	string

Value

TRUE or false

Examples

```
# numeric
    a <- numeric();                              has_multiple_levels(a)
    a <- c(1, 1);                                has_multiple_levels(a)
    a <- c(1, 2);                                has_multiple_levels(a)
# character
    a <- character();                            has_multiple_levels(a)
    a <- c('A', 'A');                            has_multiple_levels(a)
    a <- c('A', 'B');                            has_multiple_levels(a)
# factor
    a <- factor();                               has_multiple_levels(a)
    a <- factor(c('A', 'A'));                    has_multiple_levels(a)
    a <- factor(c('A', 'B'));                    has_multiple_levels(a)
# data.table
    dt <- data.table(a = factor());              has_multiple_levels(dt, 'b')
    dt <- data.table(a = factor());              has_multiple_levels(dt, 'a')
    dt <- data.table(a = factor());              has_multiple_levels(dt, 'a')
    dt <- data.table(a = factor(c('A', 'A')));   has_multiple_levels(dt, 'a')
    dt <- data.table(a = factor(c('A', 'B')));   has_multiple_levels(dt, 'a')
# sumexp
    object <- matrix(1:9, nrow = 3)
    rownames(object) <- sprintf('f%d', 1:3)
    colnames(object) <- sprintf('s%d', 1:3)
```

```
object <- list(exprs = object)
object %<>% SummarizedExperiment::SummarizedExperiment()
object$subgroup <- c('A', 'A', 'A');          has_multiple_levels(object, 'group')
object$subgroup <- c('A', 'A', 'A');         has_multiple_levels(object, 'subgroup')
object$subgroup <- c('A', 'B', 'A');         has_multiple_levels(object, 'subgroup')
```

`hdlproteins` *hdl proteomewatch proteins*

Description

hdl proteomewatch proteins

Usage

```
hdlproteins()
```

Value

string vector: HDLProteomeWatch protein entries

Examples

```
hdlproteins()
```

`impute` *Impute*

Description

Impute NA values

Usage

```
impute(object, ...)

## S3 method for class 'numeric'
impute(object, shift = 2.5, width = 0.3, verbose = TRUE, plot = FALSE, ...)

## S3 method for class 'matrix'
impute(
  object,
  shift = 2.5,
  width = 0.3,
  verbose = TRUE,
  plot = FALSE,
```

```
  n = min(9, ncol(object)),
  palette = make_colors(colnames(object)),
  ...
)

## S3 method for class 'SummarizedExperiment'
impute(
  object,
  assay = assayNames(object)[1],
  by = "subgroup",
  shift = 2.5,
  width = 0.3,
  frac = 0.5,
  verbose = TRUE,
  plot = FALSE,
  palette = make_colors(colnames(object)),
  n = min(9, ncol(object)),
  ...
)
```

Arguments

object	numeric vector, SumExp
...	required for s3 dispatch
shift	number: sd units
width	number: sd units
verbose	TRUE or FALSE
plot	TRUE or FALSE
n	number of samples to plot
palette	color vector
assay	string
by	svar
frac	fraction: fraction of available samples should be greater than this value for a subgroup to be called available

Details

Imputes NA values from N(mean - 2.5 sd, 0.3 sd)

Value

numeric vector, matrix or SumExp

Examples

```
# Simple Design
   file <- system.file('extdata/fukuda20.proteingroups.txt', package = 'autonomics')
   object <- read_maxquant_proteingroups(file)
   impute(values(object)[, 1], plot = TRUE)[1:3]              # vector
   impute(values(object),      plot = TRUE)[1:3, 1:3]         # matrix
   impute(object, plot = TRUE)                                # sumexp
# Complex Design
   subgroups <- sprintf('%s_STD', c('E00','E01','E02','E05','E15','E30','M00'))
   file <- system.file('extdata/billing19.proteingroups.txt', package = 'autonomics')
   object <- read_maxquant_proteingroups(file, subgroups = subgroups)
   impute(values(object)[1:3, 1   ])     # vector
   impute(values(object)[1:3, 1:5 ])     # matrix
   impute( object )                      # sumexp
```

---

invert_subgroups *Invert subgroups*

Description

Invert expressions , subgroups, and sample ids

Usage

```
invert_subgroups(
  object,
  subgroups = slevels(object, "subgroup"),
  sep = guess_sep(object, "subgroup")
)
```

Arguments

object	SummarizedExperiment
subgroups	character vector: subgroup levels to be inversed
sep	string: collapsed string separator

Value

character vector or SummarizedExperiment

Examples

```
file <- system.file('extdata/fukuda20.proteingroups.txt', package = 'autonomics')
object <- read_maxquant_proteingroups(file)
invert_subgroups(object)
```

is_collapsed_subset *Is collapsed subset*

Description

Is collapsed subset

Usage

```
is_collapsed_subset(x, y, sep = ";")
```

Arguments

x	character vector
y	character vector
sep	string

Value

character vector

Examples

```
x <- c(              'H3BNX8;H3BRM5', 'G5E9Y3')
y <- c('P20674;H3BNX8;H3BV69;H3BRM5', 'G5E9Y3;Q8WWN8;B4DIT1')
is_collapsed_subset(x, y)
```

is_correlation_matrix *Assert correlation matrix*

Description

Assert correlation matrix

Usage

```
is_correlation_matrix(
  x,
  .xname = get_name_in_parent(x),
  severity = getOption("assertive.severity", "stop")
)

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

Arguments

x	correlation matrix
.xname	string
severity	'warning' or 'stop'

Value

TRUE or false

Examples

```
x <- matrix(c(1,0.7, 0.3, 1), nrow = 2)
rownames(x) <- c('gene1', 'gene2')
colnames(x) <- c('gene1', 'gene2')
is_correlation_matrix(x)
is_correlation_matrix({x[1,1] <- -2; x})
```

---

is_diann_report *Is diann, fragpipe, proteingroups, phosphosites file?*

Description

Is diann, fragpipe, proteingroups, phosphosites file?

Usage

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

is_fragpipe_tsv(x, .xname = get_name_in_parent(x))

is_maxquant_proteingroups(x, .xname = get_name_in_parent(x))

is_maxquant_phosphosites(x, .xname = get_name_in_parent(x))

is_compounddiscoverer_output(x, .xname = get_name_in_parent(x))

assert_diann_report(x, .xname = get_name_in_parent(x))

assert_fragpipe_tsv(x, .xname = get_name_in_parent(x))

assert_maxquant_proteingroups(x, .xname = get_name_in_parent(x))

assert_maxquant_phosphosites(x, .xname = get_name_in_parent(x))

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

Arguments

x	file
.xname	name of x

Examples

```
file <- NULL
is_diann_report(file)
is_fragpipe_tsv(file)
is_maxquant_proteingroups(file)
is_maxquant_phosphosites(file)

file <- 3
is_diann_report(file)
is_fragpipe_tsv(file)
is_maxquant_proteingroups(file)
is_maxquant_phosphosites(file)

file <- 'blabla.tsv'
is_diann_report(file)
is_fragpipe_tsv(file)
is_maxquant_proteingroups(file)
is_maxquant_phosphosites(file)

file <- download_data('multiorganism.combined_protein.tsv')
is_diann_report(file)
is_fragpipe_tsv(file)
is_maxquant_proteingroups(file)
is_maxquant_phosphosites(file)

file <- download_data('dilution.report.tsv')
is_diann_report(file)
is_fragpipe_tsv(file)
is_maxquant_proteingroups(file)
is_maxquant_phosphosites(file)

file <- system.file('extdata/fukuda20.proteingroups.txt', package = 'autonomics')
is_diann_report(file)
is_fragpipe_tsv(file)
is_maxquant_proteingroups(file)
is_maxquant_phosphosites(file)

file <- system.file('extdata/billing19.phosphosites.txt', package = 'autonomics')
is_diann_report(file)
is_fragpipe_tsv(file)
is_maxquant_proteingroups(file)
is_maxquant_phosphosites(file)
```

is_fastadt *Is fastadt*

Description

Is fastadt

Usage

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

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

Arguments

x	fasta data.table
.xname	string

Examples

```
fastafile <- system.file('extdata/uniprot_hsa_20140515.fasta', package = 'autonomics')
x <- read_uniprotdt(fastafile)
# is_fastadt(x)  # slow
```

is_file *Is a file?*

Description

Is a file (and not a dir)

Usage

```
is_file(file)
```

Arguments

file	filepath

Details

This function distinguishies between dir and file. Others dont: is.file, fs::file_exists, assertive::is_existing_file

Examples

```
dir  <- tempdir();  dir.create(dir, showWarnings = FALSE)
file <- tempfile(); invisible(file.create(file))
is_file(dir)
is_file(file)
```

`is_fraction` *Is fraction*

Description

Is fraction

Usage

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

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

Arguments

`x`	number
`.xname`	string

Value

TRUE or false

Examples

```
is_fraction(0.1)          # YES
is_fraction(1)            # YES
is_fraction(1.2)          # NO - more than 1
is_fraction(c(0.1, 0.2))  # NO - vector
```

`is_imputed` *Get/set is_imputed*

Description

Get/Set is_imputed

Usage

```
is_imputed(object)

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

is_imputed(object) <- value

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

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

Arguments

object	SummarizedExperiment
value	matrix

Value

matrix (get) or updated object (set)

Examples

```
file <- system.file('extdata/billing19.proteingroups.txt', package = 'autonomics')
object <- read_maxquant_proteingroups(file, impute = TRUE)
sum(is_imputed(object))
```

---

is_positive_number *Is positive number*

Description

Is positive number

Usage

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

assert_positive_number(x, .xname = get_name_in_parent(x))

is_weakly_positive_number(x, .xname = get_name_in_parent(x))

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

Arguments

x	number
.xname	name of x

Value

TRUE or false

Examples

```
is_positive_number( 3)
is_positive_number(-3)
is_positive_number( 0)
is_weakly_positive_number(0)
assert_positive_number(3)
```

---

is_scalar_subset *Is scalar subset*

Description

Is scalar subset

Usage

```
is_scalar_subset(
  x,
  y,
  .xname = get_name_in_parent(x),
  .yname = get_name_in_parent(y)
)

assert_scalar_subset(
  x,
  y,
  .xname = get_name_in_parent(x),
  .yname = get_name_in_parent(y)
)
```

Arguments

x	scalar
y	SummarizedExperiment
.xname	name of x
.yname	name of y

Examples

```
file <- system.file('extdata/fukuda20.proteingroups.txt', package = 'autonomics')
object <- read_maxquant_proteingroups(file)
is_scalar_subset('subgroup',     svars(object))
is_scalar_subset('subject',      svars(object))
assert_scalar_subset('subgroup', svars(object))
```

---

is_sig *Is significant?*

Description

Is significant?

Usage

```
is_sig(
  object,
  fit = fits(object)[1],
  contrast = coefs(object),
  quantity = "fdr"
)
```

Arguments

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

Value

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

Examples

```
file <- system.file('extdata/fukuda20.proteingroups.txt', package = 'autonomics')
object <- read_maxquant_proteingroups(file)
object %<>% fit_lm()
object %<>% fit_limma()
issig <- is_sig(object, fit = c('lm','limma'), contrast = 'Adult-X30dpt')
plot_contrast_venn(issig)
```

`is_valid_formula` *Is valid formula*

Description

Is valid formula

Usage

```
is_valid_formula(
  x,
  y,
  .xname = get_name_in_parent(x),
  .yname = get_name_in_parent(y)
)

assert_valid_formula(
  x,
  y,
  .xname = get_name_in_parent(x),
  .yname = get_name_in_parent(y)
)
```

Arguments

`x`	formula
`y`	SummarizedExperiment
`.xname`	string
`.yname`	string

Value

TRUE or false

Examples

```
object <- matrix(1:9, nrow = 3)
rownames(object) <- sprintf('f%d', 1:3)
colnames(object) <- sprintf('s%d', 1:3)
object <- list(exprs = object)
object %<>% SummarizedExperiment::SummarizedExperiment()
object$group    <- 'group0'
object$subgroup <- c('A', 'B', 'C')
svars(object)
    is_valid_formula( 'condition',   object)   # not formula
    is_valid_formula( ~condition,    object)   # not svar
    is_valid_formula( ~group,        object)   # not multilevel
```

```
    is_valid_formula( ~subgroup,     object)   # TRUE
    is_valid_formula( ~0+subgroup,   object)   # TRUE
    is_valid_formula( ~1,            object)   # TRUE
assert_valid_formula( ~subgroup,     object)
```

`keep_connected_blocks` *Keep fully connected blocks*

Description

Keep fully connected blocks

Usage

```
keep_connected_blocks(object, block, verbose = TRUE)
```

Arguments

`object`	SummarizedExperiment
`block`	svar
`verbose`	TRUE or FALSE

Examples

```
file <- system.file('extdata/atkin.metabolon.xlsx', package = 'autonomics')
object <- read_metabolon(file)
object %<>% keep_connected_blocks(  block = 'Subject')
```

`keep_connected_features`
Keep features with n+ connected blocks

Description

Keep features with n+ connected blocks

Usage

```
keep_connected_features(object, block, n = 2, verbose = TRUE)
```

Arguments

`object`	SummarizedExperiment
`block`	svar
`n`	number
`verbose`	TRUE or FALSE

Examples

```
file <- system.file('extdata/atkin.metabolon.xlsx', package = 'autonomics')
object <- read_metabolon(file)
object %<>% keep_connected_blocks(  block = 'Subject')
object %<>% keep_connected_features(block = 'Subject')
```

`keep_replicated_features` *Keep replicated features*

Description

Keep features replicated for each slevel

Usage

```
keep_replicated_features(object, formula = ~1, n = 3, verbose = TRUE)
```

Arguments

`object`	SummarizedExperiment
`formula`	formula
`n`	min replications required
`verbose`	TRUE or FALSE

Examples

```
file <- system.file('extdata/atkin.metabolon.xlsx', package = 'autonomics')
object <- read_metabolon(file)
object %<>% keep_replicated_features()
object %<>% keep_replicated_features(~ subgroup)
```

`label2index` *Convert labels into indices*

Description

Convert labels into indices

Usage

```
label2index(x)
```

Arguments

`x`	‘character‘

Examples

```
label2index(x = 'Reporter intensity 0 WT(0).KD(1).OE(2).R1')
label2index(x = 'Reporter intensity 1 WT(1).KD(2).OE(3).R1')
label2index(x = 'Reporter intensity 0 WT(126).KD(127).OE(128).R1')
label2index(x = 'Reporter intensity 1 WT(126).KD(127).OE(128).R1')
label2index(x = 'Reporter intensity 1 Mix1')
```

LINMODENGINES *Linear Modeling Engines*

Description

Linear Modeling Engines

Usage

```
LINMODENGINES
```

Format

An object of class `character` of length 5.

Examples

```
LINMODENGINES
```

---

list2mat *list to matrix*

Description

list to matrix

Usage

```
list2mat(x)
```

Arguments

x	list

Value

matrix

Examples

```
x <- list(roundfruit = c('apple', 'orange'), redfruit = c('apple', 'strawberry'))
list2mat(x)
```

list_files *list files*

Description

list.files for programming

Usage

```
list_files(dir, full.names)
```

Arguments

dir	directory
full.names	TRUE or FALSE

Details

Adds a small layer on list.files. Returning NULL rather than character(0) when no files. Making it better suited for programming.

log2counts *Get/Set log2counts*

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 <- system.file('extdata/billing19.rnacounts.txt', package = 'autonomics')
object <- read_rnaseq_counts(file)
log2counts(object)[1:3, 1:3]
log2counts(object) <- values(object)
```

---

log2cpm *Get/Set log2cpm*

Description

Get / Set log2cpm matrix

Usage

```
log2cpm(object)

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

log2cpm(object) <- value

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

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

Arguments

object	SummarizedExperiment
value	log2cpm matrix (features x samples)

Value

log2cpm matrix (get) or updated object (set)

Examples

```
file <- system.file('extdata/billing19.rnacounts.txt', package = 'autonomics')
object <- read_rnaseq_counts(file)
log2cpm(object)[1:3, 1:3]
log2cpm(object) <- values(object)
```

---

log2diffs *Get/Set log2diffs*

Description

Get/Set log2diffs

Usage

```
log2diffs(object)

## S4 method for signature 'SummarizedExperiment'
log2diffs(object)

log2diffs(object) <- value

## S4 replacement method for signature 'SummarizedExperiment,matrix'
log2diffs(object) <- value

## S4 replacement method for signature 'SummarizedExperiment,numeric'
log2diffs(object) <- value
```

Arguments

object	SummarizedExperiment
value	occupancy matrix (features x samples)

Value

occpuancy matrix (get) or updated object (set)

Examples

```
file <- system.file('extdata/fukuda20.proteingroups.txt', package = 'autonomics')
object <- read_maxquant_proteingroups(file)
log2diffs(object)[1:3, 1:3]
```

log2proteins *Get/Set log2proteins*

Description

Get/Set log2proteins

Usage

```
log2proteins(object)

## S4 method for signature 'SummarizedExperiment'
log2proteins(object)

log2proteins(object) <- value

## S4 replacement method for signature 'SummarizedExperiment,matrix'
log2proteins(object) <- value

## S4 replacement method for signature 'SummarizedExperiment,numeric'
log2proteins(object) <- value
```

Arguments

object	SummarizedExperiment
value	occupancy matrix (features x samples)

Value

occpuancy matrix (get) or updated object (set)

Examples

```
file <- system.file('extdata/fukuda20.proteingroups.txt', package = 'autonomics')
object <- read_maxquant_proteingroups(file)
log2proteins(object)[1:3, 1:3]
```

log2sites *Get/Set log2sites*

Description

Get/Set log2sites

Usage

```
log2sites(object)

## S4 method for signature 'SummarizedExperiment'
log2sites(object)

log2sites(object) <- value

## S4 replacement method for signature 'SummarizedExperiment,matrix'
log2sites(object) <- value

## S4 replacement method for signature 'SummarizedExperiment,numeric'
log2sites(object) <- value
```

Arguments

object	SummarizedExperiment
value	occupancy matrix (features x samples)

Value

occpuancy matrix (get) or updated object (set)

Examples

```
file <- system.file('extdata/fukuda20.proteingroups.txt', package = 'autonomics')
object <- read_maxquant_proteingroups(file)
log2sites(object)[1:3, 1:3]
```

---

log2tpm *Get/Set log2tpm*

Description

Get / Set log2tpm matrix

Usage

```
log2tpm(object)

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

log2tpm(object) <- value

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

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

Arguments

object	SummarizedExperiment
value	log2tpm matrix (features x samples)

Value

log2tpm matrix (get) or updated object (set)

Examples

```
file <- system.file('extdata/billing19.rnacounts.txt', package = 'autonomics')
object <- read_rnaseq_counts(file)
log2tpm(object) <- values(object)
log2tpm(object)[1:3, 1:3]
```

---

log2transform *Transform values*

Description

Transform values

Usage

```
log2transform(
  object,
  assay = assayNames(object)[1],
  pseudo = 0,
  verbose = FALSE
)

exp2(object, verbose = FALSE)

zscore(object, verbose = FALSE)

sscale(mat, verbose = FALSE)

fscale(mat, verbose = FALSE)

quantnorm(object, verbose = FALSE)

invnorm(object, verbose = FALSE)

vsn(object, verbose = FALSE, delog = TRUE)
```

Arguments

object	SummarizedExperiment
assay	character vector : assays for which to perform transformation
pseudo	number : pseudo value to be added prior to transformation
verbose	TRUE or FALSE : whether to msg
mat	matrix
delog	TRUE or FALSE (vsn)

Value

Transformed sumexp

Examples

```
file <- system.file('extdata/fukuda20.proteingroups.txt', package = 'autonomics')
object <- read_maxquant_proteingroups(file)

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

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

object                       %>% plot_sample_densities()
#vsn(object)                  %>% plot_sample_densities()  # dataset too small

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

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

---

logical2factor *logical to factor*

Description

logical to factor

Usage

```
logical2factor(x, true = get_name_in_parent(x), false = paste0("not", true))

factor2logical(x)
```

Arguments

x	logical vector
true	string : truelevel
false	string : falselevel

Value

factor

Examples

```
t1up <- c( TRUE,   FALSE,  TRUE)
t1   <- c('flat', 'down', 'up' )  %>%  factor(., .)
t1up
logical2factor(t1up)
factor2logical(t1)
```

---

make_alpha_palette *Make alpha palette*

Description

Make alpha palette

Usage

```
make_alpha_palette(object, alpha)
```

Arguments

object	SummarizedExperiment
alpha	string

Value

character vector

Examples

```
file <- system.file('extdata/atkin.metabolon.xlsx', package = 'autonomics')
object <- read_metabolon(file)
make_alpha_palette(object, 'Time')
```

make_colors *Make colors*

Description

Make colors

Usage

```
make_colors(
  varlevels,
  sep = guess_sep(varlevels),
  show = FALSE,
  verbose = FALSE
)
```

Arguments

varlevels	character vector
sep	string
show	TRUE or FALSE: whether to plot
verbose	TRUE or FALSE: whether to msg

Examples

```
make_colors(c('A',   'B',   'C',  'D'  ), show = TRUE)
make_colors(c('A.1', 'B.1', 'A.2','B.2'), show = TRUE)
```

make_volcano_dt *Create volcano datatable*

Description

Create volcano datatable

Usage

```
make_volcano_dt(
  object,
  fit = fits(object)[1],
  coefs = coefs(object, fit = fit)[1],
  shape = "imputed",
  size = NULL,
  alpha = NULL,
  label = "feature_id"
)
```

Arguments

object	SummarizedExperiment
fit	'limma', 'lme', 'lm', 'wilcoxon'
coefs	character vector: coefs for which to plot volcanoes
shape	fvar or NULL
size	fvar or NULL
alpha	fvar or NULL
label	fvar or NULL

Value

data.table

Examples

```
file <- system.file('extdata/fukuda20.proteingroups.txt', package = 'autonomics')
object <- read_maxquant_proteingroups(file, impute = TRUE, fit = 'limma')
make_volcano_dt(object, fit = 'limma', coefs = 'Adult-X30dpt')
```

---

map_fvalues *Map fvalues*

Description

Map fvalues

Usage

```
map_fvalues(object, fvalues, from = "uniprot", to = "feature_id", sep = ";")
```

Arguments

object	SummarizedExperiment
fvalues	uncollapsed string vector
from	string (fvar)
to	string (svar)
sep	collapse separator

Value

string vector

Examples

```
file <- system.file('extdata/fukuda20.proteingroups.txt', package = 'autonomics')
object <- read_maxquant_proteingroups(file)
fdt(object)
map_fvalues(object, c('Q6DHL5', 'Q6PFS7'), from = 'uniprot', to = 'feature_id', sep = ';')
```

---

matrix2sumexp *Convert matrix into SummarizedExperiment*

Description

Convert matrix into SummarizedExperiment

Usage

```
matrix2sumexp(x, verbose = TRUE)
```

Arguments

x	matrix
verbose	TRUE/FALSE

Value

SummarizedExperiment

Examples

```
file <- system.file('extdata/atkin.metabolon.xlsx', package = 'autonomics')
x <- values(read_metabolon(file))
object <- matrix2sumexp(x)
object %<>% pca()
biplot(object, color = 'subgroup')
```

MAXQUANT_PATTERNS *maxquant quantity patterns*

Description

maxquant quantity patterns

Usage

```
MAXQUANT_PATTERNS
```

Format

An object of class `character` of length 7.

Examples

```
MAXQUANT_PATTERNS
```

---

mdsplot *Feature correlations/distances*

Description

Feature correlations/distances

Usage

```
mdsplot(distmat, title = NULL)

fcor(object, verbose = TRUE)

scor(object, verbose = TRUE)

fdist(object, method = "cor")

sdist(object, method = "cor")
```

Arguments

`distmat`	distance matrix
`title`	NULL or string
`object`	SummarizedExperiment
`verbose`	TRUE or FALSE
`method`	'cor', 'euclidian', etc

Value

matrix

Examples

```
# Correlations
    object <- twofactor_sumexp()
    scor(object)               %>%  pheatmap::pheatmap()
    fcor(object)               %>%  pheatmap::pheatmap()
# Distances
    sdist(object, 'cor')       %>% mdsplot('samples: cor')
    sdist(object, 'euclidian') %>% mdsplot('samples: euclidian')
```

```
fdist(object, 'cor')       %>% mdsplot('features: cor')
fdist(object, 'euclidian') %>% mdsplot('features: euclidian')
```

`merge_compounddiscoverer` *merge compound discoverer files*

Description

merge compound discoverer files

Usage

```
merge_compounddiscoverer(x, quantity = NULL, verbose = TRUE)
```

Arguments

x	'list'
quantity	''area', 'normalizedarea''
verbose	'TRUE' or 'FALSE'

Value

'data.table'

`merge_sample_excel` *Merge sample excel*

Description

Merge sample excel

Usage

```
merge_sample_excel(
  object,
  sfile,
  range = NULL,
  by.x = "sample_id",
  by.y = "sample_id"
)
```

Arguments

object	SummarizedExperiment
sfile	sample file
range	string
by.x	string
by.y	string

Value

SummarizedExperiment

---

merge_sample_file *Merge sample / feature file*

Description

Merge sample / feature file

Usage

```
merge_sample_file(
  object,
  sfile = NULL,
  by.x = "sample_id",
  by.y = "sample_id",
  all.x = TRUE,
  select = NULL,
  stringsAsFactors = FALSE,
  verbose = TRUE
)

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

Arguments

object	SummarizedExperiment
sfile	string : sample file path
by.x	string : object mergevar
by.y	string : file mergevvar
all.x	TRUE / FALSE : whether to keep samples / feature without annotation
select	character : [sf]file columns to select
stringsAsFactors	TRUE / FALSE
verbose	TRUE / FALSE
ffile	string : ffile path

Value

SummarizedExperiment

Examples

```
file <- system.file('extdata/billing19.proteingroups.txt', package = 'autonomics')
subgroups <-  c('E00','E01', 'E02','E05','E15','E30', 'M00')
subgroups %<>% paste0('_STD')
object <- read_maxquant_proteingroups(file, subgroups = subgroups)
sfile <- paste0(tempdir(),'/', basename(tools::file_path_sans_ext(file)))
sfile %<>% paste0('.samples.txt')
dt <- data.table(sample_id = object$sample_id,
                 day = split_extract_fixed(object$subgroup, '_', 1))
data.table::fwrite(dt, sfile)
sdt(object)
sdt(merge_sample_file(object, sfile))
```

---

merge_sdata *Merge sample/feature dt*

Description

Merge sample/feature dt

Usage

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

```
  verbose = TRUE
)

merge_sdt(
  object,
  dt,
  by.x = "sample_id",
  by.y = "sample_id",
  all.x = TRUE,
  verbose = TRUE
)

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

merge_fdt(
  object,
  dt,
  by.x = "feature_id",
  by.y = "feature_id",
  all.x = TRUE,
  verbose = TRUE
)
```

Arguments

object	SummarizedExperiment
dt	data.frame, data.table, DataFrame
by.x	string : object mergevar
by.y	string : df mergevar
all.x	TRUE / FALSE : whether to keep samples / features without annotation
verbose	TRUE / FALSE : whether to msg

Value

SummarizedExperiment

Examples

```
file <- system.file('extdata/atkin.metabolon.xlsx', package = 'autonomics')
object <- read_metabolon(file)
sdt(object)
```

```
sdt(merge_sdt(object, data.table(sample_id = object$sample_id,
                                 number = seq_along(object$sample_id))))
```

`message_df` *message dataframe*

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))
```

`modelvar` *Get model variable*

Description

Get model variable

Usage

```
modelvar(object, ...)

## S3 method for class 'data.table'
modelvar(
  object,
  quantity,
  fit = fits(object),
  coef = autonomics::coefs(object, fit = fit),
  ...
)

## S3 method for class 'SummarizedExperiment'
modelvar(
  object,
  quantity,
  fit = fits(object),
  coef = autonomics::coefs(object, fit = fit),
  ...
)

effectvar(
  object,
  fit = fits(object),
  coef = autonomics::coefs(object, fit = fit)
)

tvar(object, fit = fits(object), coef = autonomics::coefs(object, fit = fit))

pvar(object, fit = fits(object), coef = autonomics::coefs(object, fit = fit))

fdrvar(object, fit = fits(object), coef = autonomics::coefs(object, fit = fit))

abstractvar(object, ...)

## S3 method for class 'data.table'
abstractvar(
  object,
  fit = fits(object),
  coef = autonomics::coefs(object, fit = fit),
  ...
)

## S3 method for class 'SummarizedExperiment'
abstractvar(
  object,
  fit = fits(object),
  coef = autonomics::coefs(object, fit = fit),
```

```
  ...
)

modelvec(object, ...)

## S3 method for class 'data.table'
modelvec(
  object,
  quantity,
  fit = fits(object)[1],
  coef = autonomics::coefs(object, fit = fit)[1],
  fvar = "feature_id",
  ...
)

## S3 method for class 'SummarizedExperiment'
modelvec(
  object,
  quantity,
  fit = fits(object)[1],
  coef = autonomics::coefs(object, fit = fit)[1],
  fvar = "feature_id",
  ...
)

effectvec(
  object,
  fit = fits(object)[1],
  coef = autonomics::coefs(object)[1],
  fvar = "feature_id"
)

tvec(
  object,
  fit = fits(object)[1],
  coef = autonomics::coefs(object, fit = fit)[1],
  fvar = "feature_id"
)

pvec(
  object,
  fit = fits(object)[1],
  coef = autonomics::coefs(object, fit = fit)[1],
  fvar = "feature_id"
)

fdrvec(
  object,
```

```
  fit = fits(object)[1],
  coef = autonomics::coefs(object, fit = fit)[1],
  fvar = "feature_id"
)

abstractvec(object, ...)

## S3 method for class 'data.table'
abstractvec(
  object,
  fit = fits(object)[1],
  coef = autonomics::coefs(object, fit = fit)[1],
  fvar = "feature_id",
  ...
)

## S3 method for class 'SummarizedExperiment'
abstractvec(
  object,
  fit = fits(object)[1],
  coef = autonomics::coefs(object, fit = fit)[1],
  fvar = "feature_id",
  ...
)

modeldt(object, ...)

## S3 method for class 'data.table'
modeldt(
  object,
  quantity,
  fit = fits(object),
  coef = autonomics::coefs(object, fit = fit),
  ...
)

## S3 method for class 'SummarizedExperiment'
modeldt(
  object,
  quantity,
  fit = fits(object),
  coef = autonomics::coefs(object, fit = fit),
  ...
)

effectdt(
  object,
  fit = fits(object),
```

```
  coef = autonomics::coefs(object, fit = fit)
)

tdt(object, fit = fits(object), coef = autonomics::coefs(object, fit = fit))

pdt(object, fit = fits(object), coef = autonomics::coefs(object, fit = fit))

modelmat(
  object,
  quantity,
  fit = fits(object),
  coef = autonomics::coefs(object, fit = fit)
)

modelmat(
  object,
  quantity,
  fit = fits(object),
  coef = autonomics::coefs(object, fit = fit)
)

effectmat(
  object,
  fit = fits(object),
  coef = autonomics::coefs(object, fit = fit)
)

effectsizemat(
  object,
  fit = fits(object),
  coef = autonomics::coefs(object, fit = fit)
)

tmat(object, fit = fits(object), coef = autonomics::coefs(object, fit = fit))

pmat(object, fit = fits(object), coef = autonomics::coefs(object, fit = fit))

fdrmat(object, fit = fits(object), coef = autonomics::coefs(object, fit = fit))

modelfeatures(object, ...)

## S3 method for class 'data.table'
modelfeatures(
  object,
  fit = fits(object)[1],
  coef = autonomics::coefs(object, fit = fit)[1],
  fvar = "feature_id",
  significancevar = "p",
```

```
  significance = 0.05,
  effectdirection = "<>",
  effectsize = 0,
  ...
)

## S3 method for class 'SummarizedExperiment'
modelfeatures(object, ...)

upfeatures(
  object,
  fit = fits(object)[1],
  coef = autonomics::coefs(object, fit = fit)[1],
  fvar = "feature_id",
  significancevar = "p",
  significance = 0.05,
  effectsize = 0
)

downfeatures(
  object,
  fit = fits(object)[1],
  coef = autonomics::coefs(object, fit = fit)[1],
  fvar = "feature_id",
  significancevar = "p",
  significance = 0.05,
  effectsize = 0
)
```

Arguments

object	data.table or SummarizedExperiment
...	S3 dispatch
quantity	'p', 'effect', 'fdr', 't', or 'se'
fit	string (vector)
coef	string (vector)
fvar	'feature_id' or other fvar for values (pvec) or names (upfeatures)
significancevar	'p' or 'fdr'
significance	p or fdr cutoff (fractional number)
effectdirection	'<>', '<' or '>'
effectsize	effectsize cutoff (positive number)

Value

string (tvar), matrix (tmat), numeric vector (tvec), character vector (tfeatures)

Examples

```
file <- system.file('extdata/atkin.metabolon.xlsx', package = 'autonomics')
object <- read_metabolon(file)
object %<>% fit_limma()
object %<>% fit_lm()

effectvar(object)
effectvec(object)[1:3]
 effectdt(object)[1:3, ]
effectmat(object)[1:3, ]

     tvar(object)
     tvec(object)[1:3]
      tdt(object)[1:3, ]
     tmat(object)[1:3, ]

     pvar(object)
     pvec(object)[1:3]
      pdt(object)[1:3, ]
     pmat(object)[1:3, ]

modelfeatures(object)
 downfeatures(object)
   upfeatures(object)
```

MSIGCOLLECTIONSHUMAN *Human/Mouse Msigdb Collections*

Description

Human/Mouse Msigdb Collections

Usage

```
MSIGCOLLECTIONSHUMAN

MSIGCOLLECTIONSMOUSE
```

Format

An object of class `character` of length 25.

An object of class `character` of length 13.

MSIGDIR *local msigdb dir*

Description

local msigdb dir

Usage

```
MSIGDIR
```

Format

An object of class `character` of length 1.

nfactors *stri_split and extract*

Description

stri_split and extract

Usage

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

split_extract_fixed(x, sep, i)

split_extract_regex(x, sep, i)

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

Arguments

`x`	character vector
`sep`	string
`i`	integer

Value

character vector

Examples

```
# Read
    file <- system.file('extdata/atkin.metabolon.xlsx', package = 'autonomics')
    object <- read_metabolon(file)
    x <- object$sample_id[1:5]
    nfactors(x)
# Split
    split_extract_fixed(x, '.', 1:2)
    split_extract_fixed(x, '.', seq_len(nfactors(x)-1))
    split_extract_fixed(x, '.', nfactors(x))
    split_extract_fixed(fdt(object)$PUBCHEM, ';', 1) # with NA values
```

OPENTARGETSDIR *opentargets dir*

Description

opentargets dir

Usage

```
OPENTARGETSDIR
```

Format

An object of class `character` of length 1.

---

order_on_p *Order on p*

Description

Order on p

Usage

```
order_on_p(
  object,
  fit = autonomics::fits(object),
  coefs = autonomics::coefs(object, fit = fit),
  combiner = "|",
  decreasing = FALSE,
  verbose = TRUE
)

order_on_t(
```

```
  object,
  fit = autonomics::fits(object),
  coefs = autonomics::coefs(object, fit = fit),
  combiner = "|",
  decreasing = FALSE,
  verbose = TRUE
)

order_on_effect(
  object,
  fit = autonomics::fits(object),
  coefs = autonomics::coefs(object, fit = fit),
  combiner = "|",
  verbose = TRUE
)
```

Arguments

object	SummarizedExperiment
fit	string vector: subset of 'fits(object)'
coefs	string vector: subset of 'coefs(object)'
combiner	'|' or '&'
decreasing	TRUE or FALSE
verbose	TRUE or FALSE

Value

SummarizedExperiment

Examples

```
# Linmod
    file <- system.file('extdata/atkin.metabolon.xlsx', package = 'autonomics')
    object <- read_metabolon(file)
    order_on_p(object)
    object %<>% fit_limma()
    order_on_p(object)
# Survival
    object <- survival_example()
    object %<>% fit_survival()
    order_on_p(object)
```

pca *PCA, SMA, LDA, PLS, SPLS, OPLS*

Description

Perform a dimension reduction. Store sample scores, feature loadings, and dimension variances.

Usage

```
pca(
  object,
  by = "sample_id",
  assay = assayNames(object)[1],
  ndim = 2,
  sep = FITSEP,
  minvar = 0,
  center_samples = TRUE,
  verbose = TRUE,
  plot = FALSE,
  ...
)

pls(
  object,
  by = "subgroup",
  assay = assayNames(object)[1],
  ndim = 2,
  sep = FITSEP,
  minvar = 0,
  verbose = FALSE,
  plot = FALSE,
  ...
)

sma(
  object,
  by = "sample_id",
  assay = assayNames(object)[1],
  ndim = 2,
  sep = FITSEP,
  minvar = 0,
  verbose = TRUE,
  plot = FALSE,
  ...
)

lda(
```

```
  object,
  assay = assayNames(object)[1],
  by = "subgroup",
  ndim = 2,
  sep = FITSEP,
  minvar = 0,
  verbose = TRUE,
  plot = FALSE,
  ...
)

spls(
  object,
  assay = assayNames(object)[1],
  by = "subgroup",
  ndim = 2,
  sep = FITSEP,
  minvar = 0,
  plot = FALSE,
  ...
)

opls(
  object,
  by = "subgroup",
  assay = assayNames(object)[1],
  ndim = 2,
  sep = FITSEP,
  minvar = 0,
  verbose = FALSE,
  plot = FALSE,
  ...
)
```

Arguments

object	SummarizedExperiment
by	svar or NULL
assay	string
ndim	number
sep	string
minvar	number
center_samples	TRUE/FALSE: center samples prior to pca ?
verbose	TRUE/FALSE: message ?
plot	TRUE/FALSE: plot ?
...	passed to biplot

Value

SummarizedExperiment

Author(s)

Aditya Bhagwat, Laure Cougnaud (LDA)

Examples

```
file <- system.file('extdata/atkin.metabolon.xlsx', package = 'autonomics')
 object <- read_metabolon(file)
 pca(object, plot = TRUE)    # Principal Component Analysis
 pls(object, plot = TRUE)    # Partial Least Squares
 lda(object, plot = TRUE)    # Linear Discriminant Analysis
 sma(object, plot = TRUE)    # Spectral Map Analysis
spls(object, plot = TRUE)    # Sparse PLS
# opls(object, plot = TRUE)  # OPLS # outcommented because it produces a file named FALSE
```

---

pg_to_canonical *proteingroup to isoforms*

Description

proteingroup to isoforms

Usage

```
pg_to_canonical(x, unique = TRUE)

pg_to_isoforms(x, unique = TRUE)
```

Arguments

x	proteingroups string vector
unique	whether to remove duplicates

Value

string vector

Examples

```
 (x <- c('Q96JP5;Q96JP5-2', 'Q96JP5', 'Q96JP5-2;P86791'))
 pg_to_isoforms(x)
 pg_to_canonical(x)
 pg_to_isoforms( x, unique = FALSE)
 pg_to_canonical(x, unique = FALSE)
# .pg_to_isoforms(x[1])   # unexported dot functions
# .pg_to_canonical(x[1])  # operate on scalars
```

plot_coef_densities *Plot contrast densities*

Description

Plot contrast densities

Usage

```
plot_coef_densities(
  object,
  fit = fits(object)[1],
  coefs = autonomics::coefs(object, fit = fit),
  sep = FITSEP,
  label = "feature_id"
)
```

Arguments

object	SummarizedExperiment
fit	'limma', 'lm', 'lme', 'lmer', or 'wilcoxon'
coefs	character vector
sep	string
label	svar

Value

ggplot

Examples

```
file <- system.file('extdata/atkin.metabolon.xlsx', package = 'autonomics')
object <- read_metabolon(file)
object %<>% fit_limma(~subgroup, block = 'Subject')
plot_coef_densities(object)
```

plot_contrastogram *Plot contrastogram*

Description

Plot contrastogram

Usage

```
plot_contrastogram(
  object,
  subgroupvar,
  formula = as.formula(paste0("~ 0 +", subgroupvar)),
  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)
   plot_contrastogram(object, subgroupvar = 'subgroup')
}
```

---

plot_contrast_venn *Plot contrast venn*

Description

Plot contrast venn

Usage

```
plot_contrast_venn(issig, colors = NULL)
```

Arguments

issig	matrix(nrow, ncontrast): -1 (down), +1 (up)
colors	NULL or colorvector

Value

nothing returned

Examples

```
file <- system.file('extdata/atkin.metabolon.xlsx', package = 'autonomics')
object <- read_metabolon(file)
object %<>% fit_wilcoxon(~ subgroup, block = 'Subject')
object %<>% fit_limma(  ~ subgroup, block = 'Subject', codingfun = contr.treatment.explicit)
isfdr <- is_sig(object, contrast = 't3-t0', quantity = 'p', fit = fits(object))
plot_contrast_venn(isfdr)
```

---

plot_data *Plot data*

Description

Plot data

Usage

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

Arguments

data	data.frame'
geom	geom_point, etc.
color	variable mapped to color (symbol)
fill	variable mapped to fill (symbol)
linetype	variable mapped to linetype (symbol)
...	mapped aesthetics
palette	color palette (named character vector)
fixed	fixed aesthetics (list)
theme	list with ggplot theme specifications

Value

ggplot object

Author(s)

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Examples

```
file <- system.file('extdata/atkin.metabolon.xlsx', package = 'autonomics')
object <- read_metabolon(file)
object %<>% pca()
data <- sdt(object)
plot_data(data, x = `t~sample_id~pca1`, y = `t~sample_id~pca2`)
plot_data(data, x = `t~sample_id~pca1`, y = `t~sample_id~pca2`, color = subgroup)
plot_data(data, x = `t~sample_id~pca1`, y = `t~sample_id~pca2`, color = NULL)
fixed <- list(shape = 15, size = 3)
plot_data(data, x = `t~sample_id~pca1`, y = `t~sample_id~pca2`, fixed = fixed)
```

---

plot_densities *Plot sample/feature distributions*

Description

Plot sample/feature distributions

Usage

```
plot_densities(
  object,
  assay = assayNames(object)[1],
  group,
  fill,
  color = NULL,
  linetype = NULL,
  facet = NULL,
  nrow = NULL,
  ncol = NULL,
  dir = "h",
  scales = "free_y",
  labeller = label_value,
  palette = NULL,
  fixed = list(alpha = 0.8, na.rm = TRUE)
)

plot_sample_densities(
  object,
  assay = assayNames(object)[1],
```

```
  group = "sample_id",
  fill = if ("subgroup" %in% svars(object)) "subgroup" else "sample_id",
  color = NULL,
  linetype = NULL,
  n = 100,
  facet = NULL,
  nrow = NULL,
  ncol = NULL,
  dir = "h",
  scales = "free_y",
  labeller = label_value,
  palette = NULL,
  fixed = list(alpha = 0.8, na.rm = TRUE)
)

plot_feature_densities(
  object,
  assay = assayNames(object)[1],
  fill = "feature_id",
  group = fill,
  color = NULL,
  linetype = NULL,
  n = 9,
  facet = NULL,
  nrow = NULL,
  ncol = NULL,
  dir = "h",
  scales = "free",
  labeller = label_value,
  palette = NULL,
  fixed = list(alpha = 0.8, na.rm = TRUE)
)
```

Arguments

object	SummarizedExperiment
assay	string
group	svar (string)
fill	svar (string)
color	svar (string)
linetype	svar (string)
facet	svar (character vector)
nrow	number of facet rows
ncol	number of facet cols
dir	'h' (horizontal) or 'v' (vertical)
scales	'free', 'fixed', 'free_y'

labeller	e.g. label_value
palette	named character vector
fixed	fixed aesthetics
n	number

Value

ggplot object

See Also

plot_sample_violins, plot_sample_boxplots

Examples

```
# Data
    file <- system.file('extdata/atkin.metabolon.xlsx', package = 'autonomics')
    object <- read_metabolon(file)
    object %<>% extract(, order(.$subgroup))

# Sample distributions
    plot_sample_densities(object)
    plot_sample_violins(  object, facet = 'Time')
    plot_sample_boxplots(object)
    plot_exprs(object)
    plot_exprs(object, dim = 'samples', x = 'subgroup', facet = 'Time')

# Feature distributions
    plot_feature_densities(object)
    plot_feature_violins(  object)
    plot_feature_boxplots( object)
```

---

plot_design *Plot model*

Description

Plot model

Usage

```
plot_design(object, codingfun = contr.treatment.explicit)
```

Arguments

object	´SummarizedExperiment
codingfun	factor coding function

- contr.treatment: intercept = y0, coefi = yi - y0
- contr.treatment.explicit: intercept = y0, coefi = yi - y0
- code_control: intercept = ymean, coefi = yi - y0
- contr.diff: intercept = y0, coefi = yi - y(i-1)
- code_diff: intercept = ymean, coefi = yi - y(i-1)
- code_diff_forward: intercept = ymean, coefi = yi - y(i+)
- code_deviation: intercept = ymean, coefi = yi - ymean (drop last)
- code_deviation_first: intercept = ymean, coefi = yi - ymean (drop first)
- code_helmert: intercept = ymean, coefi = yi - mean(y0:(yi-1))
- code_helmert_forward: intercept = ymean, coefi = yi - mean(y(i+1):yp)

Value

ggplot

Examples

```
file <- system.file('extdata/billing19.proteingroups.txt', package = 'autonomics')
subgroups <- paste0(c('E00', 'E01', 'E02', 'E05', 'E15', 'E30', 'M00'), '_STD')
object <- read_maxquant_proteingroups(file, subgroups = subgroups)
object$subgroup %<>% substr(1,3)
plot_design(object)
```

---

plot_detections *Plot missingness per sample / subgroup*

Description

plot_sample_nas shows systematic and random missingness (white), and full detection (bright color) at sample resolution. Imputations are also shown (light color).

Usage

```
plot_detections(...)

plot_summarized_detections(...)

plot_sample_nas(
  object,
  by = "subgroup",
  fill = by,
  palette = make_svar_palette(object, fill),
```

```
  axis.text.y = element_blank()
)

plot_subgroup_nas(
  object,
  by = "subgroup",
  fill = by,
  palette = NULL,
  na_imputes = TRUE
)
```

Arguments

...	used to maintain deprecated functions
object	SummarizedExperiment
by	svar (string)
fill	svar (string)
palette	color vector (names = levels, values = colors)
axis.text.y	passed to ggplot2::theme
na_imputes	TRUE or FALSE

Details

plot_subgroup_nas shows systematic missingness at subgroup resolution. Random missingness and full detection are shown together (bright color). Imputations are also shown (light color).

Value

ggplot object

Examples

```
file <- system.file('extdata/fukuda20.proteingroups.txt', package = 'autonomics')
object <- read_maxquant_proteingroups(file)
plot_sample_nas(object)
plot_sample_nas(impute(object))
plot_subgroup_nas(object)
plot_subgroup_nas(impute(object))

subgroups <- sprintf('%s_STD', c('E00','E01','E02','E05','E15','E30','M00'))
file <- system.file('extdata/billing19.proteingroups.txt', package = 'autonomics')
object <- read_maxquant_proteingroups(file, subgroups = subgroups)
plot_subgroup_nas(object)
plot_subgroup_nas(object, 'subgroup')
plot_sample_nas(object)
plot_sample_nas(object, 'subgroup')
```

plot_exprs *Plot exprs for coef*

Description

Plot exprs for coef

Usage

```
plot_exprs(
  object,
  dim = "both",
  assay = assayNames(object)[1],
  features = NULL,
  fit = fits(object)[1],
  coefs = autonomics::coefs(object, fit = fit),
  block = NULL,
  x = default_x(object, dim),
  geom = default_geom(object, x = x, block = block),
  color = x,
  fill = x,
  shape = NULL,
  size = NULL,
  alpha = NULL,
  linetype = NULL,
  highlight = NULL,
  combiner = "|",
  p = 1,
  fdr = 1,
  facet = if (dim == "both") "feature_id" else NULL,
  file = NULL,
  width = 7,
  height = 7,
  n = if (is.null(file)) 4 else 12,
  ncol = if (is.null(file)) NULL else 3,
  nrow = if (is.null(file)) NULL else 4,
  scales = "free_y",
  labeller = "label_value",
  pointsize = if (is.null(block)) 0 else 0.5,
  jitter = if (is.null(block)) 0.1 else 0,
  fillpalette = make_var_palette(object, fill),
  colorpalette = make_var_palette(object, color),
  hlevels = NULL,
  title = switch(dim, both = x, features = "Feature Boxplots", samples =
    "Sample Boxplots"),
  subtitle = if (!is.null(fit)) coefs else "",
  xlab = x,
```

```
  ylab = "value",
  theme = ggplot2::theme(plot.title = element_text(hjust = 0.5)),
  verbose = TRUE
)

plot_sample_boxplots(
  object,
  fill = if ("subgroup" %in% svars(object)) "subgroup" else "sample_id",
  n = min(ncol(object), 16),
  ...
)

plot_feature_boxplots(object, ...)
```

Arguments

object	SummarizedExperiment
dim	'samples' (per-sample distribution across features), 'features' (per-feature distribution across samples) or 'both' (subgroup distribution faceted per feature)
assay	string: value in assayNames(object)
features	features to plot no matter what (character vector)
fit	'limma', 'lm', 'lme', 'lmer', 'wilcoxon'
coefs	subset of coefs(object) to consider in selecting top
block	group svar
x	x svar
geom	'boxplot' or 'point'
color	color svar: points, lines
fill	fill svar: boxplots
shape	shape svar
size	size svar
alpha	alpha svar
linetype	linetype svar
highlight	highlight svar
combiner	'&' or 'l'
p	fraction: p cutoff
fdr	fraction: fdr cutoff
facet	string: fvar mapped to facet
file	NULL or filepath
width	inches
height	inches

n	number of samples (dim = 'samples') or features (dim = 'features' or 'both') to plot
ncol	number of cols in faceted plot (if dim = 'both')
nrow	number of rows in faceted plot (if dim = 'both)
scales	'free_y', 'free'x', 'fixed'
labeller	string or function
pointsize	number
jitter	jitter width (number)
fillpalette	named character vector: fill palette
colorpalette	named character vector: color palette
hlevels	xlevels for which to plot hlines
title	string
subtitle	string
xlab	string
ylab	string
theme	ggplot2::theme(...) or NULL
verbose	TRUE or FALSE
...	used to maintain depreceated functions

Value

ggplot object

See Also

plot_sample_densities, plot_sample_violins

Examples

```
# Without limma
    file <- system.file('extdata/atkin.metabolon.xlsx', package = 'autonomics')
    object <- read_metabolon(file)
    plot_exprs(object, block = 'Subject', title = 'Subgroup Boxplots')
    plot_exprs(object, dim = 'samples')
    plot_exprs(object, dim = 'features', block = 'sample_id')
# With limma
    object %<>% fit_limma(block = 'Subject')
    plot_exprs(object, block = 'Subject')
    plot_exprs(object, block = 'Subject', coefs = c('t1-t0', 't2-t0', 't3-t0'))
    plot_exprs_per_coef(object, x = 'Time', block = 'Subject')
# Points
    plot_exprs(object, geom = 'point', block = 'Subject')
# Add highlights
    controlfeatures <- c('biotin','phosphate')
    fdt(object) %<>% cbind(control = .$feature_name %in% controlfeatures)
    plot_exprs(object, dim = 'samples', highlight = 'control')
# Multiple pages
    plot_exprs(object, block = 'Subject', n = 4, nrow = 1, ncol = 2)
```

`plot_exprs_per_coef` *Plot exprs per coef*

Description

Plot exprs per coef

Usage

```
plot_exprs_per_coef(
  object,
  fit = fits(object)[1],
  coefs = autonomics::coefs(object, fit = fit),
  x = default_x(object),
  block = NULL,
  geom = default_geom(object, x, block = block),
  orderbyp = FALSE,
  title = x,
  subtitle = default_subtitle(fit, x, coefs),
  n = 1,
  nrow = 1,
  ncol = NULL,
 theme = ggplot2::theme(legend.position = "bottom", legend.title = element_blank(),
  plot.title = element_text(hjust = 0.5), plot.subtitle = element_text(hjust = 0.5))
)
```

Arguments

`object`	SummarizedExperiment
`fit`	'limma', 'lm', 'lme', 'lmer', 'wilcoxon'
`coefs`	subset of coefs(object) to consider in selecting top
`x`	x svar
`block`	group svar
`geom`	'boxplot' or 'point'
`orderbyp`	TRUE or FALSE
`title`	string
`subtitle`	string
`n`	number
`nrow`	number of rows in faceted plot
`ncol`	number of cols in faceted plot
`theme`	ggplot2::theme(...) or NULL

Value

ggplot object

See Also

plot_sample_densities, plot_sample_violins

Examples

```
file <- system.file('extdata/atkin.metabolon.xlsx', package = 'autonomics')
object <- read_metabolon(file)
object %<>% fit_limma()
object %<>% pls(by = 'subgroup')
object %<>% pls(by = 'Diabetes')
object %<>% pls(by = 'Subject')
plot_exprs_per_coef(object)
plot_exprs_per_coef(object, orderbyp = TRUE)
plot_exprs_per_coef(object, fit = 'pls1', block = 'Subject')
```

---

plot_fit_summary *Plot fit summary*

Description

Plot fit summary

Usage

```
plot_fit_summary(sumdt, nrow = NULL, ncol = NULL, order = FALSE)
```

Arguments

sumdt	data.table
nrow	number
ncol	number
order	TRUE or FALSE

Examples

```
file <- system.file('extdata/atkin.metabolon.xlsx', package = 'autonomics')
object <- read_metabolon(file)
object %<>% fit_lm()
object %<>% fit_limma(block = 'Subject')
sumdt <- summarize_fit(object, coefs = c('t1-t0', 't2-t0', 't3-t0'))
plot_fit_summary(sumdt)
```

`plot_heatmap` *Plot heatmap*

Description

Plot heatmap

Usage

```
plot_heatmap(
  object,
  fit = fits(object)[1],
  coef = autonomics::coefs(object, fit = fit)[1],
  effectsize = 0,
  p = 1,
  fdr = 0.05,
  n = 100,
  assay = assayNames(object)[1],
  cluster_features = FALSE,
  cluster_samples = FALSE,
  flabel = intersect(c("gene", "feature_id"), fvars(object))[1],
  group = "subgroup",
  verbose = TRUE,
  title = NULL
)
```

Arguments

`object`	SummarizedExperiment
`fit`	'limma', 'lm', 'lme(r)', 'wilcoxon'
`coef`	string: one of coefs(object)
`effectsize`	number: effectsize filter
`p`	number: p filter
`fdr`	number: fdr filter
`n`	number: n filter
`assay`	string: one of assayNames(object)
`cluster_features`	TRUE or FALSE
`cluster_samples`	TRUE or FALSE
`flabel`	string: feature label
`group`	sample groupvar
`verbose`	TRUE or FALSE
`title`	string

Examples

```
file <- system.file('extdata/fukuda20.proteingroups.txt', package = 'autonomics')
object <- read_maxquant_proteingroups(file, fit = 'limma')
plot_heatmap(object)
```

`plot_joint_density` *Plot joint density*

Description

Plot joint density

Usage

```
plot_joint_density(
  object,
  xvar,
  yvar,
  color = TRUE,
  contour = TRUE,
  smooth = TRUE
)
```

Arguments

`object`	SummarizedExperiment
`xvar`	svar
`yvar`	svar
`color`	TRUE or FALSE
`contour`	TRUE or FALSE
`smooth`	TRUE or FALSE

Value

ggplot

Examples

```
file <- system.file('extdata/atkin.metabolon.xlsx', package = 'autonomics')
object <- read_metabolon(file)
set.seed(20)
object$Height <- rnorm(ncol(object), mean = 176)
object$Weight <- rnorm(ncol(object), mean = 85.4)
plot_joint_density(object, 'Height', 'Weight')
plot_joint_density(object, 'Height', 'Weight',  smooth = TRUE)
plot_joint_density(object, 'Height', 'Weight',   color = TRUE)
plot_joint_density(object, 'Height', 'Weight', contour = TRUE)
```

plot_matrix *Plot binary matrix*

Description

Plot binary matrix

Usage

```
plot_matrix(mat)
```

Arguments

mat	matrix

Value

no return (base R plot)

Examples

```
file <- system.file('extdata/atkin.metabolon.xlsx', package = 'autonomics')
object <- read_metabolon(file)
mat <- sdt(object)[, .(Subject, subgroup)]
mat$present <- 1
mat %<>% data.table::dcast(Subject ~ subgroup, value.var  = 'present', fill = 0)
mat %<>% dt2mat()
plot_matrix(mat)
```

plot_subgroup_points *Plot features*

Description

Plot features

Usage

```
plot_subgroup_points(
  object,
  subgroup = "subgroup",
  block = NULL,
  x = subgroup,
  color = subgroup,
  group = block,
  facet = "feature_id",
```

```
  nrow = NULL,
  scales = "free_y",
  ...,
  palette = NULL,
  fixed = list(na.rm = TRUE),
  theme = list(axis.text.x = element_text(angle = 90, vjust = 0.5, hjust = 1))
)
```

Arguments

object	SummarizedExperiment
subgroup	subgroup svar
block	block svar
x	svar mapped to x
color	svar mapped to color
group	svar mapped to group
facet	svar mapped to facets
nrow	number of rows
scales	'free_y' etc.
...	mapped aesthetics
palette	color palette (named character vector)
fixed	fixed aesthetics
theme	ggplot theme specifications

Value

ggplot object

Examples

```
file <- system.file('extdata/atkin.metabolon.xlsx', package = 'autonomics')
object <- read_metabolon(file, fit = 'limma')
idx <- order(fdata(object)$`p~t1-t0~limma`)[1:9]
object %<>% extract(idx, )
plot_sample_boxplots(  object)
plot_feature_boxplots( object)
plot_sample_boxplots(object, x = 'Time')
plot_subgroup_points(  object, subgroup = 'Time')
plot_subgroup_points(  object, subgroup = 'Time', block = 'Subject')
```

plot_summary *Plot summary*

Description

Plot summary

Usage

```
plot_summary(
  object,
  fit = "limma",
  formula = default_formula(object),
  block = NULL,
  label = "feature_id",
  palette = make_svar_palette(object, svar = svar)
)
```

Arguments

object	SummarizedExperiment
fit	linmod engine : 'limma', 'lm', 'lme', 'lmer' or 'wilcoxon'
formula	model formula
block	NULL or svar
label	fvar
palette	NULL or colorvector

Examples

```
file <- system.file('extdata/atkin.metabolon.xlsx', package = 'autonomics')
object <- read_metabolon(file)
object %<>% pca()
object %<>% pls(by = 'subgroup')
object %<>% fit_limma()
plot_summary(object, block = 'Subject')
```

plot_survival *Plot survival*

Description

Plot survival

Usage

```
plot_survival(
  object,
  assay = assayNames(object)[1],
  engine = intersect(fits(object), c("coxph", "survdiff", "logrank")),
  ntile = 2,
  title = sprintf("surv ~ expr"),
  subtitle = sprintf("%s", paste0(engine, collapse = "      ")),
  file = NULL,
  width = 7,
  height = 7,
  n = min(nrow(object), 9),
  ncol = 3,
  nrow = 3
)
```

Arguments

object	SummarizedExperiment
assay	value in assayNames(object)
engine	'coxph', 'survdiff' or 'logrank'
ntile	number of quantiles
title	string
subtitle	string
file	filepath
width	number
height	number
n	number of features to plot
ncol	number of columns
nrow	number of rows

Value

ggplot

Examples

```
# Defaults
    object <- survival_example()
    object %<>% fit_survival()
    plot_survival(object)
# Engines
    object <- survival_example()
    object %<>% fit_survival(engine = c('coxph', 'survdiff', 'logrank'))
    plot_survival(object)
# Pdf
    # plot_survival(object, file = file.path('testdir', 'survival', 'survival.pdf'))
```

plot_venn *Plot venn*

Description

Plot venn

Usage

```
plot_venn(x)
```

Arguments

x	list

Examples

```
x <- list(roundfruit = c('apple', 'orange'), redfruit = c('apple', 'strawberry'))
plot_venn(x)
```

plot_venn_heatmap *Plot venn heatmap*

Description

Plot venn heatmap

Usage

```
plot_venn_heatmap(x)
```

Arguments

x	list

Examples

```
x <- list(roundfruit = c('apple', 'orange'), redfruit = c('apple', 'strawberry'))
plot_venn_heatmap(x)
```

plot_violins *Plot sample/feature violins*

Description

Plot sample/feature violins

Usage

```
plot_violins(
  object,
  assay = assayNames(object)[1],
  x,
  fill,
  color = NULL,
  group = NULL,
  facet = NULL,
  nrow = NULL,
  ncol = NULL,
  dir = "h",
  scales = "free",
  labeller = label_value,
  highlight = NULL,
  palette = NULL,
  fixed = list(na.rm = TRUE)
)

plot_feature_violins(
  object,
  assay = assayNames(object)[1],
  x = "feature_id",
  fill = "feature_id",
  color = NULL,
  n = 9,
  facet = NULL,
  nrow = NULL,
  ncol = NULL,
  dir = "h",
  scales = "free",
  labeller = label_value,
  highlight = NULL,
  fixed = list(na.rm = TRUE)
)

plot_sample_violins(
  object,
  assay = assayNames(object)[1],
```

```
  x = "sample_id",
  fill = if ("subgroup" %in% svars(object)) "subgroup" else "sample_id",
  color = NULL,
  n = 100,
  facet = NULL,
  nrow = NULL,
  ncol = NULL,
  dir = "h",
  scales = "free",
  labeller = label_value,
  highlight = NULL,
  fixed = list(na.rm = TRUE)
)

plot_subgroup_violins(
  object,
  assay = assayNames(object)[1],
  subgroup,
  x = "subgroup",
  fill = "subgroup",
  color = NULL,
  highlight = NULL,
  facet = "feature_id",
  fixed = list(na.rm = TRUE)
)
```

Arguments

object	SummarizedExperiment
assay	string
x	svar (string)
fill	svar (string)
color	svar (string)
group	svar (string)
facet	svar (character vector)
nrow	NULL or number
ncol	NULL or number
dir	'h' or 'v' : are facets filled horizontally or vertically ?
scales	'free', 'free_x', 'free_y', or 'fixed'
labeller	label_both or label_value
highlight	fvar expressing which feature should be highlighted (string)
palette	named color vector (character vector)
fixed	fixed aesthetics
n	number
subgroup	subgroup svar

Value

ggplot object

See Also

plot_exprs, plot_densities

Examples

```
# data
    file <- system.file('extdata/atkin.metabolon.xlsx', package = 'autonomics')
    object <- read_metabolon(file)
    object %<>% extract(, order(.$subgroup))
    control_features <- c('biotin','phosphate')
    fdata(object) %<>% cbind(control = .$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 = 'subgroup')
```

---

plot_volcano *Plot volcano*

Description

Plot volcano

Usage

```
plot_volcano(
  object,
  fit = fits(object)[1],
  coefs = autonomics::coefs(object, fit = fit)[1],
  facet = if (is_scalar(fit)) "coef" else c("fit", "coef"),
  scales = "fixed",
  shape = if ("imputed" %in% fvars(object)) "imputed" else NULL,
  size = NULL,
  alpha = NULL,
  label = "feature_id",
  max.overlaps = 10,
  features = NULL,
  nrow = length(fit),
  p = 0.05,
  fdr = 0.05,
  n = Inf,
  xndown = NULL,
  xnup = NULL,
```

```
  title = NULL,
  file = NULL,
  width = 7,
  height = 7,
  verbose = TRUE
)
```

Arguments

object	SummarizedExperiment
fit	'limma', 'lme', 'lm', 'wilcoxon'
coefs	character vector
facet	character vector
scales	'free', 'fixed', etc.
shape	fvar (string)
size	fvar (string)
alpha	fvar (string)
label	fvar (string)
max.overlaps	number: passed to ggrepel
features	feature ids (character vector): features to encircle
nrow	number: no of rows in plot
p	number: p cutoff for labeling
fdr	number: fdr cutoff for labeling
n	number: n cutoff for labeling
xndown	x position of ndown labels
xnup	x position of nup labels
title	string or NULL
file	filename
width	number
height	number
verbose	TRUE or FALSE

Value

ggplot object

Examples

```
# Regular Usage
    file <- system.file('extdata/atkin.metabolon.xlsx', package = 'autonomics')
    object <- read_metabolon(file)
    object %<>% fit_limma()
    object %<>% fit_lm()
```

```
 plot_volcano(object, coefs = 't3-t0', fit = 'limma')                # single contrast
plot_volcano(object, coefs = c('t2-t0', 't3-t0'), fit = 'limma')     # multip contrasts
plot_volcano(object, coefs = c('t2-t0', 't3-t0'), fit = c('limma', 'lm')) # multip contrs & methods

# When nothing passes FDR
 fdt(object) %<>% add_adjusted_pvalues('fdr', fit = 'limma',coefs = 't3-t0')
 object %<>% extract( fdrvec(object, fit = 'limma', coef = 't3-t0') > 0.05, )
 plot_volcano(object, coefs = 't3-t0', fit = 'limma')

# Additional mappings
 file <- system.file('extdata/fukuda20.proteingroups.txt', package = 'autonomics')
 object <- read_maxquant_proteingroups(file, impute = TRUE)
 object %<>% fit_limma()
 plot_volcano(object)
 plot_volcano(object, label = 'gene')
 plot_volcano(object, label = 'gene', size = 'log2maxlfq')
 plot_volcano(object, label = 'gene', size = 'log2maxlfq', alpha = 'pepcounts')
 plot_volcano(object, label = 'gene', features = c('Q503D2_DANRE'))
plot_volcano(object, label = 'gene', features = list(c('Q503D2_DANRE', 'Q6DGK4_DANRE'),
                                                     c('Q6DGK4_DANRE', 'F1Q7L0_DANRE')))
```

PRECURSOR_QUANTITY *diann precursor quantity*

Description

diann precursor quantity

Usage

```
PRECURSOR_QUANTITY
```

Format

An object of class `character` of length 1.

---

preprocess_rnaseq_counts
Preprocess RNAseq counts

Description

Preprocess RNAseq counts

Usage

```
preprocess_rnaseq_counts(
  object,
  formula = ~subgroup,
  block = NULL,
  min_count = 10,
  pseudo = 0.5,
  tpm = FALSE,
  cpm = TRUE,
  voom = TRUE,
  log2 = TRUE,
  verbose = TRUE,
  plot = TRUE
)
```

Arguments

object	SummarizedExperiment
formula	designmat formula
block	blocK svar
min_count	min count required in some samples
pseudo	added pseudocount to avoid log(x)=-Inf
tpm	TRUE or FALSE : tpm normalize?
cpm	TRUE or FALSE : cpm normalize? (counts per million (scaled) reads)
voom	TRUE or FALSE : voom weight?
log2	TRUE or FALSE : log2 transform?
verbose	TRUE or FALSE : msg?
plot	TRUE or FALSE : plot?

Value

SummarizedExperiment

Examples

```
file <- system.file('extdata/billing19.rnacounts.txt', package = 'autonomics')
object <- .read_rnaseq_counts(file)
object$subgroup
object %<>% preprocess_rnaseq_counts()
```

pull_columns *Pull columns in a dataframe to the front*

Description

Pull columns in a dataframe to the front

Usage

```
pull_columns(df, first_cols, verbose = TRUE)
```

Arguments

df	data.frame
first_cols	character vector: columns to be pulled to the front
verbose	TRUE (default) or FALSE

Value

dataframe with re-ordered columns

Examples

```
df <- data.frame(
   symbol = c('A1BG', 'A2M'),
   id     = c('1',    '2'),
   name   = c('alpha-1-B glycoprotein', 'alpha-2-macroglobulin'),
   type   = c('proteincoding', 'proteincoding'))
first_cols <- c('id', 'symbol', 'location', 'uniprot')
pull_columns(df, first_cols)
```

read_affymetrix *Read affymetrix microarray*

Description

Read affymetrix microarray

Usage

```
read_affymetrix(celfiles)
```

Arguments

celfiles	string vector: CEL file paths

Value

RangedSummarizedExperiment

Examples

```
# Downloading example dataset fails 600s limit - example outcommented.
# url <- paste0('http://www.bioconductor.org/help/publications/2003/Chiaretti/chiaretti2/T33.tgz')
# localdir  <- file.path(tools::R_user_dir('autonomics', 'cache'), '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))
```

---

read_compounddiscoverer

Read compound discoverer output

Description

Read compound discoverer output

Usage

```
read_compounddiscoverer(
  dir = getwd(),
 files = list.files(path = dir, pattern = "(RP|HILIC).*\\.csv$", full.names = TRUE),
  colname_regex = "^(.*)\\d{8,8}_+(.*)_+((HILIC|RP)(NEG|POS))\\.raw.*$",
 colname_format = function(x) stringi::stri_replace_first_regex(x, colname_regex,
    "$1$2", opts_regex = stringi::stri_opts_regex(case_insensitive = TRUE)),
 mod_extract = function(x) stringi::stri_subset_regex(x, colname_regex, opts_regex =
    stringi::stri_opts_regex(case_insensitive = TRUE)) %>%
    stringi::stri_replace_first_regex(colname_regex, "$3", opts_regex =
    stringi::stri_opts_regex(case_insensitive = TRUE)),
  quantity = NULL,
  nonames = FALSE,
  exclude_sname_pattern = "(blank|QC|RS)",
  subgroups = NULL,
  logbase = 2,
  impute = FALSE,
  plot = FALSE,
  label = "feature_id",
  pca = plot,
  pls = plot,
```

```
  fit = if (plot) "limma" else NULL,
  formula = ~subgroup,
  block = NULL,
  coefs = NULL,
  contrasts = NULL,
  palette = NULL,
  verbose = TRUE
)
```

Arguments

dir	compound discoverer output directory
files	compound discoverer output files
colname_regex	regular expression to parse sample names from column names
colname_format	function to reformat column names
mod_extract	function to extract MS modi from sample names
quantity	'area', 'normalizedarea' or NULL
nonames	TRUE or FALSE: retain compunds without Names?
exclude_sname_pattern	regular expression of sample names to exclude
subgroups	NULL or string vector : subgroups to retain
logbase	base for logarithmization of the data
impute	TRUE or FALSE: impute group-specific NA values?
plot	TRUE or FALSE: plot ?
label	fvar
pca	TRUE or FALSE: run pca ?
pls	TRUE or FALSE: run pls ?
fit	model engine: 'limma', 'lm', 'lme(r)', 'wilcoxon' or NULL
formula	model formula
block	model blockvar: string or NULL
coefs	model coefficients of interest: character vector or NULL
contrasts	coefficient contrasts of interest: character vector or NULL
palette	color palette : named character vector
verbose	TRUE or FALSE : message ?

Value

SummarizedExperiment

read_fragpipe *Read fragpipe*

Description

Read fragpipe

Usage

```
read_fragpipe(
  dir = getwd(),
  file = if (is_file(dir)) dir else file.path(dir, "combined_protein.tsv"),
  contaminants = FALSE,
  verbose = TRUE
)
```

Arguments

dir	directory with 'combined_protein.tsv'
file	'combined_protein.tsv' (full path)
contaminants	whether to include contaminants
verbose	whether to msg

Value

SummarizedExperiment

Examples

```
file <- download_data('multiorganism.combined_protein.tsv')
object <- read_fragpipe(file = file)
object
fdt(object)
sdt(object)
```

read_maxquant_phosphosites *Read maxquant phosphosites*

Description

Read maxquant phosphosites

Usage

```
read_maxquant_phosphosites(
  dir = getwd(),
  fosfile = if (is_file(dir)) dir else file.path(dir, "phospho (STY)Sites.txt"),
  profile = file.path(dirname(fosfile), "proteinGroups.txt"),
  fastafile = NULL,
  restapi = FALSE,
  quantity = NULL,
  subgroups = NULL,
  invert = character(0),
  rm_contaminants = TRUE,
  rm_reverse = TRUE,
  rm_missing_in_all_samples = TRUE,
  localization = 0.75,
  impute = FALSE,
  plot = FALSE,
  label = "feature_id",
  pca = plot,
  pls = plot,
  fit = if (plot) "limma" else NULL,
  formula = as.formula("~ subgroup"),
  block = NULL,
  coefs = NULL,
  contrasts = NULL,
  palette = NULL,
  verbose = TRUE
)

read_phosphosites(...)
```

Arguments

dir	proteingroups directory
fosfile	phosphosites file
profile	proteingroups file
fastafile	uniprot fastafile
restapi	TRUE or FALSE : annotate non-fastadt uniprots using uniprot restapi
quantity	'normalizedratio', 'ratio', 'correctedreporterintensity', 'reporterintensity', 'maxlfq', 'labeledintensity', 'intensity' or NULL
subgroups	NULL or string vector : subgroups to retain
invert	string vector: subgroups which require inversion
rm_contaminants	TRUE or FALSE: rm contaminants ?
rm_reverse	TRUE or FALSE: rm reverse proteins ?
rm_missing_in_all_samples	TRUE or FALSE

localization	number: min localization probability (for phosphosites)
impute	TRUE or FALSE: impute group-specific NA values?
plot	TRUE or FALSE
label	fvar
pca	TRUE or FALSE: run pca ?
pls	TRUE or FALSE: run pls ?
fit	model engine: 'limma', 'lm', 'lme(r)', 'wilcoxon' or NULL
formula	model formula
block	model blockvar: string or NULL
coefs	model coefficients of interest: string vector or NULL
contrasts	model coefficient contrasts of interest: string vector or NULL
palette	color palette: named string vector
verbose	TRUE or FALSE: message ?
...	maintain deprecated functions

Value

SummarizedExperiment

Examples

```
  profile <- system.file('extdata/billing19.proteingroups.txt', package = 'autonomics')
  fosfile <- system.file('extdata/billing19.phosphosites.txt',  package = 'autonomics')
fastafile <- system.file('extdata/uniprot_hsa_20140515.fasta',  package = 'autonomics')
subgroups <- sprintf('%s_STD', c('E00', 'E01', 'E02', 'E05', 'E15', 'E30', 'M00'))
pro <- read_maxquant_proteingroups(file = profile, subgroups = subgroups)
fos <- read_maxquant_phosphosites(fosfile = fosfile, profile = profile, subgroups = subgroups)
fos <- read_maxquant_phosphosites(fosfile = fosfile, profile = profile, fastafile = fastafile, subgroups = subgroup
```

---

read_maxquant_proteingroups

Read maxquant proteingroups

Description

Read maxquant proteingroups

Usage

```
read_maxquant_proteingroups(
  dir = getwd(),
  file = if (is_file(dir)) dir else file.path(dir, "proteinGroups.txt"),
  fastafile = NULL,
  restapi = FALSE,
  quantity = NULL,
  subgroups = NULL,
  invert = character(0),
  rm_contaminants = TRUE,
  rm_reverse = TRUE,
  rm_missing_in_all_samples = TRUE,
  impute = FALSE,
  plot = FALSE,
  label = "feature_id",
  pca = plot,
  pls = plot,
  fit = if (plot) "limma" else NULL,
  formula = as.formula("~ subgroup"),
  block = NULL,
  coefs = NULL,
  contrasts = NULL,
  palette = NULL,
  verbose = TRUE
)

read_proteingroups(...)
```

Arguments

dir	proteingroups directory
file	proteingroups file
fastafile	uniprot fastafile
restapi	TRUE or FALSE : use uniprot restapi to annotate uniprots not in fastadt ?
quantity	'normalizedratio', 'ratio', 'correctedreporterintensity', 'reporterintensity', 'maxlfq', 'labeledintensity', 'intensity' or NULL
subgroups	NULL or string vector : subgroups to retain
invert	string vector : subgroups which require inversion
rm_contaminants	TRUE or FALSE : rm contaminants ?
rm_reverse	TRUE or FALSE : rm reverse proteins ?
rm_missing_in_all_samples	TRUE or FALSE
impute	TRUE or FALSE: impute group-specific NA values?
plot	TRUE or FALSE: plot ?

label	fvar
pca	TRUE or FALSE: run pca ?
pls	TRUE or FALSE: run pls ?
fit	model engine: 'limma', 'lm', 'lme(r)', 'wilcoxon' or NULL
formula	model formula
block	model blockvar: string or NULL
coefs	model coefficients of interest: character vector or NULL
contrasts	coefficient contrasts of interest: character vector or NULL
palette	color palette : named character vector
verbose	TRUE or FALSE : message ?
...	maintain deprecated functions

Value

SummarizedExperiment

Examples

```
# fukuda20 - LFQ
    file <- system.file('extdata/fukuda20.proteingroups.txt', package = 'autonomics')
    pro <- read_maxquant_proteingroups(file = file)

# billing19 - Normalized Ratios
       file <- system.file('extdata/billing19.proteingroups.txt', package = 'autonomics')
   fastafile <- system.file('extdata/uniprot_hsa_20140515.fasta', package = 'autonomics')
    subgroups <- sprintf('%s_STD', c('E00', 'E01', 'E02', 'E05', 'E15', 'E30', 'M00'))
    pro <- read_maxquant_proteingroups(file = file, subgroups = subgroups)
   pro <- read_maxquant_proteingroups(file = file, fastafile = fastafile, subgroups = subgroups)
```

---

read_msigdt *Read msigdb datatable*

Description

Read msigdb datatable

Usage

```
read_msigdt(
  file = list_files(MSIGDIR, full.names = TRUE)[1],
 collections = if (is.null(file)) NULL else switch(basename(file) %>% substr(nchar(.)
  - 4, nchar(.) - 3), Hs = c("C2:CP:REACTOME", "C5:GO:BP", "C5:GO:MF", "C5:GO:CC"), Mm
    = c("M2:CP:REACTOME", "M5:GO:BP", "M5:GO:MF", "M5:GO:CC"))
)
```

Arguments

file	msigdb file: one of the files in dir(MSIGDB).
collections	subset of names(MSIGCOLLECTIONS)

Examples

```
read_msigdt()
```

---

read_olink *Read olink file*

Description

Read olink file

Usage

```
read_olink(file, sample_excel = NULL, sample_tsv = NULL, by.y = "SampleID")
```

Arguments

file	olinkfile
sample_excel	sample excel
sample_tsv	sample tsv
by.y	sample tsv mergeby column

Value

SummarizedExperiment

Examples

```
# Example data
    npxdt   <- data.table::data.table(OlinkAnalyze::npx_data1)[, c(1:11, 17)]
    sampledt <- data.table::data.table(OlinkAnalyze::npx_data1)[, c(1, 12:15)]
    sampledt %<>% extract(!grepl('CONTROL', SampleID))
    sampledt %<>% unique()
# Write to file
    file <- paste0(tempfile(), '.olink.csv')
    samplefile <- paste0(tempfile(), '.samples.xlsx')
    data.table::fwrite(npxdt, file)
    writexl::write_xlsx(sampledt, samplefile)
# Read
    object <- read_olink(file, sample_excel = samplefile)
    biplot(pca(object), color = 'Time', group = 'Subject', shape = 'Treatment')
```

read_salmon *Read salmon*

Description

Read salmon

Usage

```
read_salmon(dir, sfile = NULL, by = NULL, ensdb = NULL)
```

Arguments

dir	salmon results rootdir
sfile	samplefile
by	samplefile column to merge by
ensdb	EnsDb object

Value

SummarizedExperiment

Examples

```
# dir <- '../bh/salmon_quants'
# sfile <- '../bh/samplesheet.csv'
# by <- 'salmonDir'
# ah <- AnnotationHub::AnnotationHub()
# ensdb <- ah[['AH98078']]
# read_salmon(dir, sfile = sfile, by = 'salmonDir', ensdb = ensdb)
```

read_uniprotdt *Read fasta hdrs*

Description

Read fasta hdrs

Usage

```
read_uniprotdt(fastafile, fastafields = FASTAFIELDS, verbose = TRUE)

parse_maxquant_hdrs(fastahdrs)

read_contaminantdt(force = FALSE, verbose = TRUE)
```

Arguments

fastafile	string (or charactervector)
fastafields	charactervector : which fastahdr fields to extract ?
verbose	bool
fastahdrs	character vector
force	whether to overwrite existing file

Value

data.table(uniprot, protein, gene, uniprot, reviewed, existence)

Note

existence values are always those of the canonical isoform (no isoform-level resolution for this field)

Examples

```
# uniprot hdrs
    fastafile <- system.file('extdata/uniprot_hsa_20140515.fasta', package = 'autonomics')
     read_uniprotdt(fastafile)

# maxquant hdrs
    file <- system.file('extdata/fukuda20.proteingroups.txt', package = 'autonomics')
    dt <- .read_maxquant_proteingroups(file)
    parse_maxquant_hdrs(dt$`Fasta headers`)

   profile <- system.file('extdata/billing19.proteingroups.txt', package = 'autonomics')
   fosfile <- system.file('extdata/billing19.phosphosites.txt',  package = 'autonomics' )
    prodt <- .read_maxquant_proteingroups(profile)
    fosdt <- .read_maxquant_phosphosites(fosfile, profile)
    parse_maxquant_hdrs(prodt$`Fasta headers`)
    parse_maxquant_hdrs(fosdt$`Fasta headers`)

# contaminant hdrs
    read_contaminantdt()
```

---

reexports *Objects exported from other packages*

Description

These objects are imported from other packages. Follow the links below to see their documentation.

data.table data.table

magrittr %<>%, %>%, extract

reset_fit *Reset fit*

Description

Reset fit

Usage

```
reset_fit(
  object,
  fit = fits(object),
  coefs = autonomics::coefs(object, fit = fit),
  verbose = TRUE
)
```

Arguments

object	SummarizedExperiment
fit	character vector
coefs	character vector
verbose	TRUE or FALSE

Examples

```
file <- system.file('extdata/atkin.metabolon.xlsx', package = 'autonomics')
(object <- read_metabolon(file))
object %<>% reset_fit()
object %<>% fit_limma() %>% reset_fit()
object %<>% fit_limma() %>% fit_lm() %>% reset_fit()
object %<>% fit_limma() %>% fit_lm() %>% reset_fit('limma')
```

rm_diann_contaminants *Rm contaminants*

Description

Rm contaminants from DIA-NN SumExp

Usage

```
rm_diann_contaminants(object, verbose = TRUE)
```

Arguments

object	SummarizedExperiment
verbose	TRUE or FALSE

Value

SummarizedExperiment

Examples

```
file <- download_data('dilution.report.tsv')
object <- read_diann_proteingroups(file)
object %<>% rm_diann_contaminants()
```

---

rm_missing_in_all_samples

Rm features missing in some samples

Description

Rm features missing in some samples

Usage

```
rm_missing_in_all_samples(object, verbose = TRUE)

rm_missing_in_some_samples(object, verbose = TRUE)
```

Arguments

object	SummarizedExperiment
verbose	TRUE (default) or FALSE

Value

updated object

Examples

```
file <- system.file('extdata/atkin.metabolon.xlsx', package = 'autonomics')
object <- read_metabolon(file)
rm_missing_in_all_samples( object)
rm_missing_in_some_samples(object)
```

`rm_unmatched_samples` *rm unmatched/singleton samples*

Description

rm unmatched/singleton samples

Usage

```
rm_unmatched_samples(
  object,
  subgroupvar = "subgroup",
  subgroupctr = slevels(object, subgroupvar)[1],
  block,
  verbose = TRUE
)

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

Arguments

`object`	SummarizedExperiment
`subgroupvar`	subgroup variable (string)
`subgroupctr`	control subgroup (string)
`block`	block variable (string)
`verbose`	TRUE/FALSE

Value

SummarizedExperiment

Examples

```
file <- system.file('extdata/atkin.somascan.adat', package = 'autonomics')
object <- read_somascan(file)
object %<>% filter_samples(subgroup %in% c('t1', 't2'), verbose = TRUE)
rm_singleton_samples(object, subgroupvar = 'Subject')
rm_unmatched_samples(object, subgroupvar = 'subgroup', block = 'Subject')
```

scaledlibsizes *Get tmm-scaled libsizes*

Description

Get tmm-scaled libsizes

Usage

```
scaledlibsizes(counts)
```

Arguments

counts	counts matri

Value

scaled libsize vector

Examples

```
file <- system.file('extdata/billing19.rnacounts.txt', package = 'autonomics')
object <- read_rnaseq_counts(file)
scaledlibsizes(counts(object))
```

scoremat *Extract scores/loadings*

Description

Extract scores/loadings

Usage

```
scoremat(object, method = "pca", by = biplot_by(object, method), dim = 1:2)

scores(object, method = "pca", by = biplot_by(object, method), dim = 1)

loadingmat(object, method = "pca", by = biplot_by(object, method), dim = 1:2)

loadings(object, method = "pca", by = biplot_by(object, method), dim = 1)
```

Arguments

object	SummarizedExperiment
method	'pca', 'pls', etc.
by	svar (string)
dim	numeric vector

Examples

```
file <- system.file('extdata/atkin.metabolon.xlsx', package = 'autonomics')
object <- read_metabolon(file)
object %<>% pca()
    scores(object)[1:2]
  loadings(object)[1:2]
  scoremat(object)[1:2, ]
loadingmat(object)[1:2, ]
```

---

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 <- system.file('extdata/billing19.proteingroups.txt', package = 'autonomics')
object <- read_maxquant_proteingroups(file)
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

```
file <- system.file('extdata/billing19.proteingroups.txt', package = 'autonomics')
object <- read_maxquant_proteingroups(file)
head(snames(object))
head(snames(object) %<>% paste0('SAMPLE_', .))
```

split_samples *Split samples*

Description

Split samples by svar

Usage

```
split_samples(object, by = "subgroup")

cbind_imputed(objlist)

split_features(object, by)
```

Arguments

object	SummarizedExperiment
by	svar to split by (string)
objlist	SummarizedExperiment list

Value

SummarizedExperiment list

Examples

```
file <- system.file('extdata/atkin.metabolon.xlsx', package = 'autonomics')
object <- read_metabolon(file)
objlist <- split_features(object, by = 'PLATFORM')
objlist <- split_samples(object, 'Diabetes')
objlist %<>% Map(impute, .)
object <- cbind_imputed(objlist)
```

---

stri_any_regex *Does any string have a regex*

Description

Does any string have a regex

Usage

```
stri_any_regex(str, pattern)
```

Arguments

str	string vector
pattern	string

Value

TRUE or FALSE

Examples

```
str <- c('s1 Spectral Count', 's1 Unique Spectral Count')
patterns <- c('Spectral Count', '(?<!Unique) Spectral Count', 'Intensity')
stringi::stri_detect_regex(str, pattern = patterns[1])
stringi::stri_detect_regex(str, pattern = patterns[2])
stringi::stri_detect_regex(str, pattern = patterns[3])
stri_any_regex(   str, pattern = patterns)
```

---

stri_detect_fixed_in_collapsed

Detect fixed patterns in collapsed strings

Description

Detect fixed patterns in collapsed strings

Usage

```
stri_detect_fixed_in_collapsed(x, patterns, sep)
```

Arguments

x	vector with collapsed strings
patterns	vector with fixed patterns (strings)
sep	collapse separator (string) or NULL (if uncollapsed)

Value

boolean vector

Examples

```
file <- system.file('extdata/fukuda20.proteingroups.txt', package = 'autonomics')
object <- read_maxquant_proteingroups(file)
x <- fdt(object)$uniprot
patterns <- c('A0A0R4IKT8', 'Q7T3G6')
table(stri_detect_fixed_in_collapsed(x = x, patterns = patterns, sep = ';'))
```

subgroup_array *Get subgroup matrix*

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 <- system.file('extdata/atkin.metabolon.xlsx', package = 'autonomics')
object <- read_metabolon(file)
object$subgroup <- paste0(object$Diabetes, '.', object$subgroup)
subgroup_matrix(object, 'subgroup')
```

subtract_baseline *Subtract baseline*

Description

Subtract baseline level within block

Usage

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

```
subtract_pairs(
  object,
  subgroupvar = "subgroup",
  subgroupctr = slevels(object, subgroupvar)[1],
  block,
  assaynames = assayNames(object)[1],
  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
    file <- system.file('extdata/atkin.metabolon.xlsx', package = 'autonomics')
    object0 <- read_metabolon(file)
    pca(object0, plot = TRUE, color = 'Time')

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

# subtract_pairs: optimized for many blocks
    object <- subtract_pairs(object0, block = 'Subject', subgroupvar = 'Time')
```

```
    pca(object, plot = TRUE, color = 'Time')

# subtract_differences
    object <- subtract_differences(object0, block = 'Subject', subgroupvar = 'Time')
    values(object) %<>% na_to_zero()
    pca(object, plot = TRUE, color = 'Time')
```

`sumexplist_to_longdt` *SummarizedExperiment list to long data.table*

Description

SummarizedExperiment list to long data.table

Usage

```
sumexplist_to_longdt(
  sumexplist,
  svars = intersect("subgroup", autonomics::svars(sumexplist[[1]])),
  fvars = intersect("gene", autonomics::fvars(sumexplist[[1]])),
  setvarname = "set"
)
```

Arguments

`sumexplist`	list of SummarizedExperiments
`svars`	character vector
`fvars`	character vector
`setvarname`	string

Value

data.table

Examples

```
subgroups <- paste0(c('E00', 'E01', 'E02', 'E05', 'E15', 'E30', 'M00'), '_STD')
rnafile <- system.file('extdata/billing19.rnacounts.txt',     package = 'autonomics')
profile <- system.file('extdata/billing19.proteingroups.txt', package = 'autonomics')
fosfile <- system.file('extdata/billing19.phosphosites.txt',  package = 'autonomics')
rna <- read_rnaseq_counts(rnafile)
pro <- read_maxquant_proteingroups(file = profile, subgroups = subgroups)
fos <- read_maxquant_phosphosites(fosfile = fosfile, profile = profile, subgroups = subgroups)
pro$subgroup %<>% stringi::stri_replace_first_fixed('_STD', '')
fos$subgroup %<>% stringi::stri_replace_first_fixed('_STD', '')

sumexplist <- list(rna = rna, pro = pro, fos = fos)
dt <- sumexplist_to_longdt(sumexplist, setvarname = 'platform')
dt %<>% extract(gene %in% c('TNMD', 'TSPAN6'))
```

sumexp_to_tsv *Write sumexp to tsv*

Description

Write sumexp to tsv

Usage

```
sumexp_to_tsv(object, assay = assayNames(object)[1], file)
```

Arguments

object	SummarizedExperiment
assay	string
file	filename

Examples

```
file <- system.file('extdata/fukuda20.proteingroups.txt', package = 'autonomics')
object <- read_maxquant_proteingroups(file, fit = 'limma')
tsv <- file.path(tempdir(), 'fukuda20.proteingroups.tsv')
sumexp_to_tsv(object, file = tsv)
```

sumexp_to_widedt *SummarizedExperiment to data.table*

Description

SummarizedExperiment to data.table

Usage

```
sumexp_to_widedt(
  object,
  fvars = autonomics::fvars(object),
  assay = assayNames(object)[1]
)

sumexp_to_longdt(
  object,
  fvars = intersect("feature_name", autonomics::fvars(object)),
  svars = intersect("subgroup", autonomics::svars(object)),
  assay = assayNames(object) %>% intersect(c(.[1], "is_imputed"))
)

sumexp_to_subrep_dt(object, subgroup = subgroup)
```

Arguments

object	sumexp
fvars	additional fvars to include in table
assay	matrix in assays(object) to be used
svars	additional svars to include in table
subgroup	subgroup (sym)

Details

- sumexp_to_widedt: feature x sample
- sumexp_to_subrep_dt: feature.subgroup x replicate
- sumexp_to_longdt: feature.sample

Value

data.table

Examples

```
# Atkin Hypoglycemia
   file <- system.file('extdata/atkin.metabolon.xlsx', package = 'autonomics')
   object <- read_metabolon(file)
   sumexp_to_widedt(object)
   sumexp_to_longdt(object)
   sumexp_to_subrep_dt(object)

# Fukuda
   file <- system.file('extdata/fukuda20.proteingroups.txt', package = 'autonomics')
   object <- read_maxquant_proteingroups(file)
   values(object)
   fdt(object)
   object %<>% impute()
   table(fdt(object)$imputed)
   sumexp_to_longdt(object)
   sumexp_to_widedt(object)
   sumexp_to_longdt(object)
```

---

summarize_fit *Summarize fit*

Description

Summarize fit

Usage

```
summarize_fit(object, ...)

## S3 method for class 'data.table'
summarize_fit(
  object,
  fit = fits(object),
  coefs = autonomics::coefs(object, fit = fit),
  ...
)

## S3 method for class 'SummarizedExperiment'
summarize_fit(
  object,
  fit = fits(object),
  coefs = autonomics::coefs(object, fit = fit),
  ...
)
```

Arguments

object	SummarizedExperiment or data.table
...	S3 dispatch
fit	'limma', 'lme', 'lm', 'lme', 'wilcoxon' or NULL
coefs	string vector

Value

data.table(contrast, nup, ndown)

Examples

```
file <- system.file('extdata/atkin.metabolon.xlsx', package = 'autonomics')
object <- read_metabolon(file)
object %<>% fit_limma()
object %<>% fit_lm()
summarize_fit(object, coefs = c('t1-t0', 't2-t0', 't3-t0'))
```

SURVIVALENGINES *Survival engines*

Description

Survival engines

Usage

```
SURVIVALENGINES
```

Format

An object of class `character` of length 3.

Examples

```
SURVIVALENGINES
```

`survival_example` *Fit survival*

Description

Investigates association between expression and survival

Usage

```
survival_example()

fit_survival(
  object,
  ntile = 2,
  engine = c("survdiff", "coxph", "logrank")[1:2],
  assay = assayNames(object)[1],
  sep = FITSEP,
  verbose = TRUE,
  outdir = NULL,
  plot = if (is.null(outdir)) FALSE else TRUE,
  width = 7,
  height = 7,
  n = min(nrow(object), 9),
  ncol = 3,
  nrow = 3,
  writefunname = "write_xl"
)
```

Arguments

`object`	SummarizedExperiment
`ntile`	number
`engine`	'coxph' (survival), 'survdiff' (survival), 'logrank' (coin)
`assay`	string
`sep`	fvar string separator : e.g. '~' gives p~surv~LR50

verbose	TRUE or FALSE
outdir	dir
plot	TRUE or FALSE
width	number
height	number
n	number of features to plot
ncol	number of cols
nrow	number of rows
writefunname	'write_xl' or 'write_ods'

Details

Investigates association between expression and survival.
Continuous for coxph.
Categorical for survdiff or logrank
Samples are split into ntile expression groups.
Survival is compared between highest and lowest expressors.

Three statistics recorded per engine
p
effect: coef (coxph)
mean survival difference (survdiff, logrank)
t: z (coxph)
χ^2 (survdiff, logrank)
sign reflects whether expression
increases (positive) or decreases (negative) survival

Value

SummarizedExperiment

Examples

```
# Defaults
    object <- survival_example()
    fit_survival(object)
# Engines
    fit_survival(object, engine = c('coxph', 'survdiff'))
    fit_survival(object, engine = c('coxph', 'survdiff', 'logrank'))
# Quantiles
    fit_survival(object, engine = 'logrank')
    fit_survival(object, engine = 'logrank', ntile = 4)
# Plot
    fit_survival(object)
    fit_survival(object, plot = TRUE)
    fit_survival(object, engine = c('coxph', 'survdiff', 'logrank'), plot = TRUE)
```

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 <- system.file('extdata/billing19.proteingroups.txt', package = 'autonomics')
object <- read_maxquant_proteingroups(file)
svalues(object, 'subgroup')
subgroup_values(object)
```

svars *Get/Set svars*

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 fector with variable names

Value

sample variable names (get) or updated SummarizedExperiment

Examples

```
file <- system.file('extdata/billing19.proteingroups.txt', package = 'autonomics')
object <- read_maxquant_proteingroups(file)
svars(object)[1]
(svars(object)[1] %<>% paste0('1'))
```

---

systematic_nas *Is systematic/random/full NA*

Description

Is systematic/random/full NA

Usage

```
systematic_nas(object, by = "subgroup", frac = 0.5)

random_nas(object, by = "subgroup")

no_nas(object)
```

Arguments

object	SummarizedExperiment
by	svar (string)
frac	fraction

Examples

```
file <- system.file('extdata/fukuda20.proteingroups.txt', package = 'autonomics')
object <- read_maxquant_proteingroups(file)
table(systematic_nas(object))   # missing in some subgroups, present in others
table(random_nas(object))       # missing in some samples, independent of subgroup
table(no_nas(object))           # missing in no samples
```

---

tag_features *Tag features*

Description

Tag features

Usage

```
tag_features(
  object,
  keyvar,
  sep,
  features,
  tagvar = get_name_in_parent(features),
  verbose = TRUE
)
```

Arguments

object	SummarizedExperiment
keyvar	string : intersection fvar
sep	string : keyvar collapse separator
features	character vector : intersection set
tagvar	string :
verbose	TRUE or FALSE

Value

SummarizedExperiment

Examples

```
file <- system.file('extdata/atkin.somascan.adat', package = 'autonomics')
object <- read_somascan(file)
features <- AnnotationDbi::keys(org.Hs.eg.db::org.Hs.eg.db, keytype = 'SYMBOL')
object %<>% tag_features(keyvar = 'EntrezGeneSymbol', sep = ' ', features)
table(fdt(object)$features)
```

---

tag_hdlproteins *Tag hdlproteins*

Description

Tag hdlproteins

Usage

```
tag_hdlproteins(object, verbose = TRUE)
```

Arguments

object	SummarizedExperiment
verbose	TRUE or FALSE

Value

SummarizedExperiment

Examples

```
file <- system.file('extdata/billing19.proteingroups.txt', package = 'autonomics')
object <- read_maxquant_proteingroups(file)
object %<>% tag_hdlproteins()
fdt(object)
```

TAXON_TO_ORGNAME *Annotation Maps*

Description

Annotation Maps

Usage

```
TAXON_TO_ORGNAME

ABBREV_TO_ORGNAME

REVIEWED_TO_NUMBER

EXISTENCE_TO_NUMBER
```

Format

An object of class `character` of length 7.

An object of class `character` of length 4.

An object of class `character` of length 2.

An object of class `numeric` of length 4.

Examples

```
    TAXON_TO_ORGNAME['9606']
   ABBREV_TO_ORGNAME['HSA']
 REVIEWED_TO_NUMBER['reviewed']
EXISTENCE_TO_NUMBER['Evidence at protein level']
```

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

twofactor_sumexp *twofactor sumexp*

Description

twofactor sumexp

Usage

```
twofactor_sumexp()
```

Value

SummarizedExperiment

uncollapse *Uncollapse/Recollapse*

Description

Uncollapse data.table cols

Usage

```
uncollapse(dt, ..., sep = ";")

recollapse(dt, by, sep = ";")
```

Arguments

dt	data.table
...	cols
sep	string
by	string

Examples

```
# Example data
   (dt <- data.table::data.table(
              uniprot  = 'Q9BQL6;Q96AC1;Q96AC1-3',
              protein  = 'FERM1_HUMAN;FERM2_HUMAN',
              gene     = 'FERMT1;FERMT2',
              family   = 'FERM'))
# Uncollapse
    uncollapse(dt, protein, gene, sep = ';')
    recollapse( uncollapse(dt, protein, gene, sep = ';'), by = 'uniprot')
```

```
# Unchanged when no sep
    uncollapse(dt, family, sep = ';')
    uncollapse(dt, family, sep = 'NOSEP')
```

---

values *Get/Set expr values*

Description

Get/Set value matrix

Usage

```
values(object)

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

values(object) <- value

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

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

Arguments

object	SummarizedExperiment
value	ratio matrix (features x samples)

Value

value matrix (get) or updated object (set)

Examples

```
file <- system.file('extdata/billing19.proteingroups.txt', package = 'autonomics')
object <- read_maxquant_proteingroups(file)
values(object)[1:3, 1:3]
values(object) <- 0
values(object)[1:3, 1:3]
```

varlevels_dont_clash *Are varlevels unique*

Description

Are varlevels unique

Usage

```
varlevels_dont_clash(object, ...)

## S3 method for class 'data.table'
varlevels_dont_clash(object, vars = names(object), ...)

## S3 method for class 'SummarizedExperiment'
varlevels_dont_clash(object, vars = svars(object), ...)
```

Arguments

object	SummarizedExperiment or data.table
...	required for s3 dispatch
vars	character vector

Value

TRUE or FALSE

Examples

```
require(data.table)
object1 <- data.table(expand.grid(genome = c('WT', 'MUT'), treat = c('control', 'drug')))
object2 <- data.table(expand.grid(mutant = c('YES', 'NO'), treated = c('YES', 'NO')))
varlevels_dont_clash(object1)
varlevels_dont_clash(object2)
```

venn_detects *Venn detects*

Description

Venn diagram full/consistent/random detects

Usage

```
venn_detects(object, by = "subgroup")
```

Arguments

object	SummarizedExperiment
by	svar (string)

Value

NULL

Examples

```
file <- system.file('extdata/fukuda20.proteingroups.txt', package = 'autonomics')
object <- read_maxquant_proteingroups(file)
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
...	addtional params
value	ratio matrix (features x samples)

Value

weight matrix (get) or updated object (set)

Examples

```
file <- system.file('extdata/billing19.rnacounts.txt', package = 'autonomics')
object <- read_rnaseq_counts(file)
weights(object)[1:3, 1:2]
weights(object) <- 1
weights(object)[1:3, 1:2]
```

---

write_xl *Write xl/ods*

Description

Write xl/ods

Usage

```
write_xl(
  object,
  xlfile,
  fitcoefs = autonomics::fitcoefs(object),
  verbose = TRUE
)

write_ods(
  object,
  odsfile,
  fitcoefs = autonomics::fitcoefs(object),
  verbose = TRUE
)
```

Arguments

object	SummarizedExperiment
xlfile	file
fitcoefs	character vector
verbose	TRUE or FALSE
odsfile	file

Value

filepath

Examples

```
file <- system.file('extdata/atkin.metabolon.xlsx', package = 'autonomics')
object <- read_metabolon(file, fit = 'limma')
xlfile  <- file.path(tempdir(), 'fukuda20.proteingroups.fdt.xlsx')
odsfile <- file.path(tempdir(), 'fukuda20.proteingroups.fdt.ods')
# write_xl(object,  xlfile)
# write_ods(object, odsfile)
```

X *Model based prediction*

Description

Model based prediction

Usage

```
X(
  object,
  formula = default_formula(object),
  drop = varlevels_dont_clash(object, all.vars(formula)),
  codingfun = contr.treatment.explicit
)

beta(object, fit = fits(object)[1])
```

Arguments

object	SummarizedExperiment or data.frame
formula	formula
drop	TRUE or FALSE
codingfun	function
fit	'limma', 'lm', 'lme', 'wilcoxon'

Value

beta matrix (nlevel x nfeature)

Examples

```
file <- system.file('extdata/atkin.metabolon.xlsx', package = 'autonomics')
object <- read_metabolon(file)
object %<>% fit_limma(block = 'Subject') # intercept required!
beta(object)                    #    betas : nlevel x nfeature
   X(object)                    #   design : nlevel x nlevel
   X(object) %*% beta(object)   # response : nlevel x nfeature
```

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)

na_to_string(x)
```

Arguments

x	matrix
verbose	logical(1)

Value

Updated matrix

Examples

```
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