Package 'InteRact'

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Description The InteRact package provides tools to analyse affinity purification data
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add_GO_data add_Hallmark_data add_KEGG_data analyse_interactome annotation_enrichment_analysis append_annotations append_FDR append_PPI average_technical_replicates compute_correlations compute_FDR_from_asymmetry create_summary_table_PPI discretize_values dot_plot 10

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add_GO_data

Add GO annotations

Description

Add GO annotations corresponding to a set of protein identifiers

Usage

```
add_GO_data(df, map_id = "Entry", GO_type = "molecular_function",
  organism = "mouse", slim = FALSE, updateProgress = NULL)
```

add_Hallmark_data 3

Arguments

df a data.frame with protein IDs in column map_id
map_id column name used to map protein identifiers

GO_type type of GO term ("molecular_function", "biological_process" or "cellular_component")

organism organism for which the annotations have to be mapped

slim logical, use GO_slim annotations

updateProgress logical, function to show progress in shiny app

Value

a data.frame with an additional GO annotation column

Description

Add Hallmark annotations corresponding to a set of protein identifiers

Usage

```
add_Hallmark_data(df, map_id = "Gene.names...primary..",
    updateProgress = NULL)
```

Arguments

df a data.frame with protein IDs in column map_id
map_id column name used to map protein identifiers
updateProgress logical, function to show progress in shiny app

Value

a data.frame with an additional Hallmark annotation column

add_KEGG_data Add KEGG pathway annotations

Description

Add KEGG pathway annotations corresponding to a set of KEGG IDs

Usage

```
add_KEGG_data(df, map_id = "Cross.reference..KEGG.", organism = "mouse",
    updateProgress = NULL)
```

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Arguments

df a data.frame with KEGG IDs in column map_id

map_id column name used to map KEGG IDs

organism organism for which the annotations have to be mapped

updateProgress logical, function to show progress in shiny app

Value

a data.frame with an additional KEGG pathway annotation column

across experimental conditions

Description

Construct an interactome by comparing bait and control background across experimental conditions

Usage

```
analyse_interactome(df, ibait, bait_gene_name, Npep, Protein.IDs, name_bait,
  name_ctrl, background, conditions, replicates, by_conditions = TRUE,
  pool_background = TRUE, log_test = TRUE, log_stoichio = TRUE,
  substract_ctrl = TRUE)
```

Arguments

df a data frame of protein intensities. columns are experimental samples and rows

are proteins

ibait : row index corresponding to the bait protein

bait_gene_name : The gene name of the bait

Npep : vector containing the number of theoretically observable peptide per protein

(same length as dim(df)[1])

Protein.IDs : vector containing protein IDs (same length as dim(df)[1])

name_bait : name of the bait as appearing in the background vector

name_ctrl : name of the control as appearing in the background vector

background : vector of background names for each experimental sample

conditions : vector of conditions for each each experimental sample

replicates : vector of biological replicates for each each experimental sample

by_conditions option to perform the comparison between bait and control group for each con-

dition

pool_background

option to use all control background conditions as one control group for all

conditions

log_test logical, perform t-test on log transform intensities

log_stoichio logical, use the geometric mean instead of the arithmetic mean to compute stoi-

chiometries

substract_ctrl logical, substract ctrl intensities in the calculation of stoichiometries

Value

```
an object of class InteRactome, i.e a list including the following elements:
conditions: a vector of experimental conditions.

names: a vector of names (by default gene names are used).

p_val: a list of vectors containing the p values associated to each experimental condition.

fold_change: a list of vectors containing the fold change associated to each experimental condition.

...: other variables.
```

```
annotation_enrichment_analysis

Perform enrichment analysis
```

Description

Perform enrichment analysis for protein annotations stored in a formatted data.frame

Usage

```
annotation_enrichment_analysis(df, idx_detect,
  annotation_selected = c("Keywords", "Protein.families"),
  names = df$Gene.names...primary.., organism = "mouse",
  updateProgress = NULL, showProgress = TRUE, orderOutput = TRUE)
```

Arguments

df a formatted data.frame with annoations corresponding to each row. Types of

annotations are organized by columns.

idx_detect indexes of the foreground set.

annotation_selected

set of annotations on which to perform the analysis

names row names. Used in the output data.frame

organism organism for which the analysis is to be performed ("mouse" or "human")

updateProgress logical, function to show progress in shiny app

showProgress logical, show progress in console

orderOutput logical, order annotations by enrichment p-values in the output data.frame

Value

a data.frame

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append_annotations

Append annotations to an InteRactome

Description

Append annotations to an InteRactome

Usage

```
append_annotations(res, annotations = NULL, name_id = "Protein.IDs",
  organism = "mouse")
```

Arguments

res an InteRactome

annotations type of annotations to append

name_id column name used to map protein identifiers

organism organism for which the annotations have to be appended

Value

an InteRactome

append_FDR

Append a FDR column to an InteRactome

Description

Append a FDR column to an InteRactome

Usage

```
append_FDR(res, df)
```

Arguments

res an InteRactome

df a data.frame containing (at least) columns 'bait', names', 'FDR' and 'condi-

tions'

Value

an InteRactome

append_PPI 7

Examples

```
# #load data :
data("proteinGroups_Cbl")
#Run InteRact with default parameters
res <- InteRact(proteinGroups_Cbl, bait_gene_name = "Cbl")$Interactome
df_merge <- merge_conditions(res)
df_FDR <- compute_FDR_from_asymmetry(df_merge)
Interactome <- append_FDR(res, df_FDR)</pre>
```

append_PPI

Append protein-protein interaction

Description

Append protein-protein interaction information to an InteRactome. PPI are retrieved from databases IntAct, MINT, BioGRID and HPRD

Usage

```
append_PPI(res, mapping = "names")
```

Arguments

res an InteRactome

mapping name of the InteRactome's variable containing gene names

Value

an InteRactome

```
average_technical_replicates
```

Average protein intensities over technical replicates

Description

Average protein intensities over technical replicates

Usage

```
average_technical_replicates(df, cond, log = TRUE)
```

Arguments

df A data frame of protein intensities

cond A data frame containing the description of df's columns (i.e "idx", bckg", "time",

"bio" and "tech") as returned by function identify_conditions()

log use geometric mean

Value

A list containing:

Intensity, a data frame of protein intensities averaged over technical replicates; conditions, a data frame containing the description of Intensity's columns

Examples

```
#load data :
data("proteinGroups_Cbl")
cond <- identify_conditions(proteinGroups_Cbl)
Column_intensity_pattern <- "^Intensity."
df_int <- proteinGroups_Cbl[ , grep(Column_intensity_pattern, colnames(df))]</pre>
```

compute_correlations Compute correlation in protein recruitment

Description

Compute correlation in protein recruitment from interaction stoichiometries computed across all conditions for each biological replicate. Pearson correlations are used.

Usage

```
compute_correlations(res, idx = NULL)
```

Arguments

res an InteRactome

idx indexes of the set of proteins for which correlations will be computed

Value

a data.frame with protein correlation information (correlation coefficient in column 'r_corr' and associated p-value in column 'p-corr')

```
compute_FDR_from_asymmetry
```

Compute the FDR from the asymmetry of the volcano plot

Description

Compute the FDR (False Discovery Rate) using the asymmetry of the volcano plot. It uses the fonction f(x) = c / (x-x0) with $x = log10(fold_change)$, $y=-log10(p_value)$. Points with x>x0 and y>f(x) are taken as true positive (TP) Points with x<x0 and y>f(x) are taken as false positive (FP) For a given set of parameters (c,x0), the FDR is given by TP/(TP+FP)

Usage

```
compute_FDR_from_asymmetry(df, c = seq(from = 0, to = 4, by = 0.1), x0 = seq(from = 0, to = 3, by = 0.1))
```

Arguments

df : a data.frame containing columns p_val and fold_change

c : numeric vector x0 : numeric vector

Value

a data.frame with a extra column FDR.

If parameters c and x0 are vectors, FDR is taken as the minimum FDR value across all sets of parameters

Examples

```
# #load data :
data("proteinGroups_Cb1")
#Run InteRact with default parameters
res <- InteRact(proteinGroups_Cb1, bait_gene_name = "Cb1")$Interactome
df_merge <- merge_conditions(res)
df_FDR <- compute_FDR_from_asymmetry(df_merge)
Interactome <- append_FDR(res, df_FDR)</pre>
```

```
create_summary_table_PPI
```

Retrieve protein-protein interaction information from databses IntAct, MINT, BioGRID and HPRD

Description

Retrieve protein-protein interaction information from databses IntAct, MINT, BioGRID and HPRD

Usage

```
create_summary_table_PPI(gene_name)
```

Arguments

gene_name the gene name for which to retrieve PPI

Value

a data.frame PPI information

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discretize_values

Discretize values in a vector based on a finite set of values

Description

Discretize values in a vector based on a finite set of values

Usage

```
discretize_values(x, breaks = c(1, 0.1, 0.05, 0.01),
  decreasing_order = TRUE)
```

Arguments

x numeric vector

breaks numeric vector. Set of discrete values on which x values will be mapped. Non-

mapped values will be set to NA

decreasing_order

logical. Map beaks values from the greatest to the smallest

Value

a numeric vector

 dot_plot

Dot plot representation of matrices

Description

Dot plot representation of matrices

Usage

```
dot_plot(Dot_Size, Dot_Color = NULL, title = "Dot Plot",
    size_range = range(Dot_Size), size_var = "size", color_var = "color")
```

Arguments

Dot_Size a matrix of dot sizes

Dot_Color a matrix of dot colors (optionnal)

title plot title

size_range range of dot sizes to display

size_var name of the variable corresponding to dot size color_var name of the variable corresponding to dot color

Value

a plot

estimate_Npep 11

estimate_Npep

Get the number of theoretically observable peptides per protein

Description

Get the number of theoretically observable peptides per protein

Usage

```
estimate_Npep(df, Column_Npep = NULL)
```

Arguments

df A data frame

Column_Npep column containing the number of theoretically observable peptides per protein.

If NULL try to compute the number of theoretically observable peptides using

iBAQ values, or use molecular weight.

Value

A data frame with the column 'Npep'

filter_conditions

Filter conditions from an interactome

Description

Filter conditions from an interactome

Usage

```
filter_conditions(res, conditions_to_filter_out)
```

Arguments

```
res an InteRactome conditions_to_filter_out
```

character vector with names of conditions to filter out

Value

an InteRactome

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filter_Proteins	Filtering of a data frame using a threshold on protein identification
	score and gene names

Description

Filtering of a data frame using a threshold on protein identification score and gene names

Usage

```
filter_Proteins(df, min_score = 0, Column_gene_name = "Gene.names",
   Column_score = "Score", split_param = ";")
```

Arguments

df A data frame

min_score Threshold for protein identification score

Column_gene_name

The name of df's column containing gene names

Column_score The name of df's column containing protein identification score

split_param Character used to split gene names into substrings.

Value

A filtered data frame. Contains an extra column with the first substring of the column Column_gene_name

geom_mean	Perform the geometric mean of a numeric vector
-----------	--

Description

Perform the geometric mean of a numeric vector

Usage

```
geom_mean(x, na.rm = TRUE)
```

Arguments

x A numeric vector na.rm remove NA values

Value

A numeric value

get_annotations 13

get_annotations Get annotations from uniprot for a set of protein identifiers

Description

Get annotations from uniprot for a set of protein identifiers. From a set of IDs, keep the first that correspond to a "reviewed" protein, or by default the first ID of the set name_id: column containing the set of protein identifiers separated by "split_param" organism = c("mouse", "human")

Usage

```
get_annotations(data, name_id = "Protein.IDs", split_param = ";",
  organism = "mouse", updateProgress = NULL)
```

Arguments

data a data.frame with protein IDs in column name_id
name_id column name used to map protein identifiers

split_param split character used to separate different protein IDs organism organism for which the annotations have to be appended

updateProgress logical, function to show progress in shiny app

Value

an InteRactome

get_PPI_from_BioGRID Retrieve protein-protein interaction information from BioGRID

Description

Retrieve protein-protein interaction information from BioGRID

Usage

```
get_PPI_from_BioGRID(gene_name, tax_ID = c(9606, 10090))
```

Arguments

gene_name the gene name for which to retrieve PPI tax_ID taxon ID for which to retrieve PPI

Value

a data.frame PPI information

get_PPI_from_HPRD

Retrieve protein-protein interaction information from HPRD

Description

Retrieve protein-protein interaction information from HPRD

Usage

```
get_PPI_from_HPRD(gene_name)
```

Arguments

gene_name

the gene name for which to retrieve PPI

get_PPI_from_psicquic Retrieve protein-protein interaction information using PSICQUIC

Description

Retrieve protein-protein interaction information using PSICQUIC

Usage

```
get_PPI_from_psicquic(gene_name, tax_ID = c(9606, 10090),
    provider = c("IntAct", "MINT"))
```

Arguments

gene_name the gene name for which to retrieve PPI

tax_ID taxon ID for which to retrieve PPI
provider database from which to retrieve PPI

Value

a data.frame PPI information

15 global_analysis

global_analysis Adds global variables by analysing values acro- InteRactome	y analysing values across all conditions of an
--	--

Description

Adds global variables by analysing values across all conditions of an InteRactome

Usage

```
global_analysis(res)
```

Arguments

res an InteRactome

Value

an InteRactome with global varaiables

identify_conditions	Identify conditions (background, time of stimulation, biological and
	technical replicates) from column names

Description

Identify conditions (background, time of stimulation, biological and technical replicates) from column names

Usage

```
identify_conditions(df, Column_intensity_pattern = "^Intensity.",
  split = "_", bckg_pos = 1, bio_pos = 2, time_pos = 3, tech_pos = 4)
```

Arguments

df	A dataframe containing protein intensities. By default, protein intensity col-
	umn names start by "Intensity." (use parameter Column_intensity_pattern to
	change)

Column_intensity_pattern

Pattern (regular exrpression) used to identfy df's columns containing protein

intensity values

split Character used to split column names into substrings Position of the sample background in splitted column names bckg_pos Position of the sample biological replicate in splitted column names bio_pos time_pos Position of the sample experimental condition in splitted column names Position of the sample technical replicate in splitted column names tech_pos

16 identify_interactors

Value

a data frame describing experimental samples in terms of background, biological and technical replicates, and experimental conditions

Examples

```
#load data :
data("proteinGroups_Cbl")
# You can identify columns and their description separately using \code{identify_conditions()}
cond <- identify_conditions(proteinGroups_Cbl)
print.data.frame(cond)
# and use it as parameters for function InteRact()
res <- InteRact(proteinGroups_Cbl, bait_gene_name = "Cbl", condition = cond)$Interactome</pre>
```

Description

Identify specific interactors in an InteRactome

Usage

```
identify_interactors(res, var_p_val = "p_val", p_val_thresh = 0.05,
  fold_change_thresh = 2, n_success_min = 1, consecutive_success = FALSE,
    ...)
```

Arguments

res an InteRactome

var_p_val name of the p-value variable

p_val_thresh p-value threshold

fold_change_thresh fold-change threshold

n_success_min minimal number of conditions in which the interactor must pass the the p-value and the fold-change thresholds

consecutive_success logical, impose that the interactor must pass selection thresholds in n_success_min

consecutive conditions.

... additionnal paramters passed to function order_interactome()

Value

an InteRactome with extra variables is_interactor, n_success and interactor

InteRact 17

InteRact	Analysis of AP-MS data	

Description

Analysis of AP-MS data

Usage

```
InteRact(df, updateProgress = NULL, N_rep = 3, quantile_rep = 0.05,
  pool_background = TRUE, log_test = TRUE, log_stoichio = TRUE,
  log_mean = TRUE, by_conditions = TRUE, substract_ctrl = TRUE,
  preprocess_df = NULL, ...)
```

Arguments

df A dataframe containing protein intensities. By default, protein intensity col-

umn names start by "Intensity." (use parameter Column_intensity_pattern to

change)

updateProgress function to show progress bar in shiny app

N_rep Number of iterations for the replacement of missing values

quantile_rep Numeric value between 0 and 1. Quantile of the distribution of mean intensities

in the control background used to replace missing values.

pool_background

option to use all control background conditions as one control group for all

conditions

log_test logical, perform t-test on log transform intensities

log_stoichio logical, use the geometric mean instead of the arithmetic mean to compute stoi-

chiometries

log_mean logical, use the geometric mean instead of the arithmetic mean to compute the

mean InteRactome

by_conditions option to perform the comparison between bait and control group for each con-

dition

substract_ctrl logical, substract ctrl intensities in the calculation of stoichiometries

preprocess_df list obtained by the function preprocess_data()

... Additional parameters passed to function preprocess_data() and identify_conditions

Value

a list containing the preprocessed data and on object of class InteRactome, i.e a list including the following elements:

conditions: a vector of experimental conditions.

names: a vector of names (by default gene names are used).

p_val: a list of vectors containing the p values associated to each experimental condition.

fold_change : a list of vectors containing the fold change associated to each experimental condition.

...: other variables.

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Author(s)

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Examples

```
#load data :
data("proteinGroups_Cbl")
#Run InteRact with default parameters
res <- InteRact(proteinGroups_Cbl, bait_gene_name = "Cbl")$Interactome</pre>
#You now have an \code{InteRactome}. See its elements.
class(res)
names(res)
#Generate volcano plots
plot_volcanos(res)
#Identify specific interactors
res <- identify_interactors(res, p_val_thresh = 0.05, fold_change_thresh = 2)</pre>
#Visualize interaction kinetics
plot_per_condition(res)
# Append protein abundance information
res <- merge_proteome(res)</pre>
# Append annotations
annot <- get_annotations(res)</pre>
res <- append_annotations(res,</pre>
                                 annot)
#Create a summary data frame
sum_tbl <- summary_table(res)</pre>
```

mean_analysis

Compute the mean InteRactome (on variables 'p_val', 'fold_cahnge', 'stoichio' and 'stoichio_bio') from a list of InteRactomes

Description

Compute the mean InteRactome (on variables 'p_val', 'fold_cahnge', 'stoichio' and 'stoichio_bio') from a list of InteRactomes

Usage

```
mean_analysis(res, log = TRUE, na.rm = TRUE)
```

Arguments

res a list of InteRactome

logical, use the geometric mean instead of the arithmetic mean

na.rm logical, remove NA values

merge_conditions 19

merge_conditions	Merge different conditions from different interactomes into a single
	data.frame

Description

Merge different conditions from different interactomes into a single data.frame

Usage

```
merge_conditions(res, selected_conditions = NULL)
```

Arguments

```
res a list of InteRactomes
selected_conditions
a character vector containing names of conditions to merge
```

Value

a data.frame with columns bait, names, Protein.IDs, conditions, p_val, fold_change

```
merge_duplicate_groups
```

Merge protein groups with the same gene name.

Description

Merge protein groups with the same gene name.

Usage

```
merge_duplicate_groups(df, idx_col = NULL, merge_column = "gene_name")
```

Arguments

df A data frame

idx_col idx of columns for which values will be merged across protein groups

merge_column column to identify rows to be be merged

Value

A merged data frame

20 moving_average

merge_proteome

Add protein abundance to an InteRactome

Description

Add protein abundance to an InteRactome. Protein abundance are obtained from CD4+ effector T cells.

Usage

```
merge_proteome(res)
```

Arguments

res

an InteRactome

moving_average

Performs a running average on a numeric vector

Description

Performs a running average on a numeric vector

Usage

```
moving_average(x, n)
```

Arguments

x a numeric vector

n integer, radius of the moving avergae (number of points extending on each side

of the center point on which the average is computed)

Value

a smoothed numeric vector

order_interactome 21

order_interactome

Order proteins within an InteRactome

Description

Order proteins within an InteRactome

Usage

```
order_interactome(res, var_p_val = "min_p_val", p_val_breaks = c(1, 0.1, 0.05, 0.01))
```

Arguments

res an InteRactome

var_p_val name of the p-value variable

p_val_breaks numeric vector to discretize p-value

Value

an InteRactome

plot_2D_stoichio

Plot abundance versus interaction stoichiometries

Description

Plot abundance versus interaction stoichiometries

Usage

```
plot_2D_stoichio(res, condition = "max", xlim = NULL, ylim = NULL,
    N_display = 30)
```

Arguments

res an InteRactome

condition condition selected. If "max", the maximum stoichiometry across conditions will

be used.

xlim range of x values ylim range of y values

N_display maximum number of protein to display

Value

a plot

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```
plot_annotation_results
```

Plot the result of the annotation enrichment analysis

Description

Plot the result of the annotation enrichment analysis

Usage

```
plot_annotation_results(df, p_val_max = 0.05, method_adjust_p_val = "fdr",
    fold_change_min = 2, N_annot_min = 2)
```

Arguments

```
df a formatted data.frame obtained by the function annotation_enrichment_analysis()

p_val_max threshold for the enrichment p-value

method_adjust_p_val
    method to adjust p-value for multiple comparisons

fold_change_min
    threshold for the enrichment fold-change

N_annot_min minimum number of elements that are annotated in the foreground set
```

Value

a plot

plot_comparison

Plot protein intensities per biological replicate and background

Description

Plot protein intensities per biological replicate and background

Usage

```
plot_comparison(res, name, conditions, textsize = 3, test = "t.test",
  test.args = list(paired = FALSE), map_signif_level = c(*** = 0.001, **
  = 0.01, * = 0.05), position = "position_jitter",
  position.args = list(width = 0.3, height = 0))
```

Arguments

res an InteRactome

name name of the protein to display conditions set of conditions to display

textsize size of labels corresponding to significance levels

test name of the test function to compare intensities between background

test.args arguments passed to function test

map_signif_level

named vector with labels and corresponding significance levels

position name of the function used to position data points

position.args arguments passed to function position

Value

a plot

plot_correlation_network

Plot an interactive correlation network with communities highlighted

Description

Plot an interactive correlation network with communities highlighted

Usage

```
plot_correlation_network(df_corr, r_corr_thresh = 0.8, p_val_thresh = 0.05)
```

Arguments

df_corr a data.frame with columns 'r_corr' and 'p_corr'

r_corr_thresh threshold for variable 'r_corr' (min)
p_val_thresh threshold for ariable 'p_corr' (max)

Value

an interactive networkD3 plot

24 plot_per_condition

plot_per_condition	Dot plot representation of interaction as a function of experimental conditions
--------------------	---

Description

Dot plot representation of interaction as a function of experimental conditions

Usage

```
plot_per_condition(res, idx_cols = 1:length(res$conditions),
  idx_rows = 1:20, size_var = "norm_stoichio", size_range = c(0, 1),
  color_var = "p_val", color_breaks = c(1, 0.1, 0.05, 0.01),
  color_default = 1, save_file = NULL, plot_width = 2.5 +
  length(res$conditions)/5, plot_height = 2 + length(idx_rows)/5,
  clustering = TRUE)
```

Arguments

res	an InteRactome
idx_cols	numeric vector to select and order conditions to be displayed
idx_rows	numeric vector to select proteins to display
size_var	name of the variable corresponding to dot size
size_range	range of dot sizes to display
color_var	name of the variable corresponding to dot color
color_breaks	vector used to discretize colors
color_default	value corresponding to the default color
save_file	path of output file (.pdf)
plot_width	width of the output .pdf file
plot_height	height of the output .pdf file
clustering	logical or numeric vector. If logical, use hierarchical clustering to order proteins. If numeric, ordering indexes for displayed proteins (must be the same length as idx_rows)

Value

```
a list conataining :
a plot "plot"
a numeric vector "idx_order" containing the position of the protein displayed within the InteRactome
```

plot_QC 25

plot_QC

Quality check plots for preprocessed AP-MS data

Description

Quality check plots for preprocessed AP-MS data

Usage

```
plot_QC(prep_data)
```

Arguments

prep_data

preprocessed data as obtained using function preprocess_data()

Value

Several QC plots

plot_stoichio

Plot interaction stoichiometries per biological replicate

Description

Plot interaction stoichiometries per biological replicate

Usage

```
plot_stoichio(res, name, conditions = res$conditions,
  ref_condition = res$conditions[1], test = "t.test",
  test.args = list(paired = TRUE), map_signif_level = c(*** = 0.001, **
  = 0.01, * = 0.05), save_file = NULL)
```

Arguments

res an InteRactome

name name of the protein to display conditions set of conditions to display

ref_condition name of the reference condition for all test

test name of the test function to compare sttoichiometries between conditions

test.args arguments passed to function test

map_signif_level

named vector with labels and corresponding significance levels

save_file path of output file (.pdf)

Value

a plot

26 preprocess_data

plot_volcanos

Plot protein enrichement fold-change versus p-value

Description

Plot protein enrichement fold-change versus p-value

Usage

```
plot_volcanos(res, labels = NULL, N_print = 15, conditions = NULL,
    p_val_thresh = 0.05, fold_change_thresh = 2, save_file = NULL,
    xlim = NULL, ylim = NULL, asinh_transform = TRUE)
```

Arguments

res an InteRactome

labels for proteins in plot. Must the same length as res\$names

N_print maximum of protein labels to display

conditions conditions to plot

p_val_thresh threshold on p-value to display

fold_change_thresh

threshold on fold-change to display

save_file path of output file (.pdf)

xlim range of x values ylim range of y values

asinh_transform

logical, display asinh(log10(p-value)) on the y-axis

Value

a plot

preprocess_data

Preprocessing of raw data

Description

Preprocessing of raw data

Usage

```
preprocess_data(df, Column_gene_name = "Gene.names", Column_score = "Score",
   Column_ID = "Protein.IDs", Column_Npep = NULL,
   Column_intensity_pattern = "^Intensity.", bait_gene_name,
   condition = NULL, bckg_bait = bait_gene_name, bckg_ctrl = "WT",
   log = TRUE, filter_time = NULL, filter_bio = NULL, filter_tech = NULL,
   ...)
```

proteinGroups_Cbl 27

Arguments

df Data.frame with protein intensities

Column_gene_name

Column with gene names

Column_score Column with protein identification score

Column_ID Column with protein IDs

Column_Npep Column with number of theoretically observable peptides per protein

Column_intensity_pattern

Pattern (regular expression) used to identfy df's columns containing protein

intensity values

bait_gene_name The gene name of the bait

condition data.frame with columns "sample", bckg", "bio", "time" and "tech" indicating

for each intensity column ("sample") its corresponding background ("bckg"), biological replicate ("bio), experimental condition ("tine) and technical replicate

("tech).

bckg_bait Name of the bait background as found in condition\$bckg (see below)
bckg_ctrl Name of the control background as found in condition\$bckg (see below)

log logical, use geometric mean to average technical replicates filter_time vector of experimental conditions to exclude from analysis filter_bio vector of biological replicates to exclude from analysis filter_tech vector of technical replicates to exclude from analysis

... Additional parameters passed to function identify_conditions

proteinGroups_Cbl Characterization of protein groups identified from AP-MS data using

MaxQuant

Description

A dataset containing the characterization of protein groups identified using MaxQuant from AP-MS samples. Samples correspond to pull-down experiments performed on Cd4+ T cells from CBL-OST mice (expressing a tagged version of the bait protein Cbl) and WT mice (expressing the endogeneous Cbl protein). Cd4+ T cells from CBL-OST and WT backgrounds were stimulated by crosslinking of Cd3e and Cd4 for different times (0, 30, 120, 300 and 600 seconds). Samples were then lysed and subjected to MS-MS analysis. Experiments were conducted in three biological replicates (S1, S2 and S3). Sample were analysed by MS-MS in three technical replicates (R1, R2 and R3).

Usage

proteinGroups_Cbl

Format

A data frame with 1978 rows (protein groups) and 849 variables:

See the Maxquant documentation for the description of the different variables

28 row_mean

rescale_median

Normalize data frame by columns using the median

Description

Normalize data frame by columns using the median

Usage

```
rescale_median(df)
```

Arguments

df

A data frame

Value

A normalized data frame

row_mean

Compute the mean by row

Description

Compute the mean by row

Usage

```
row_mean(df, na.rm = TRUE, log = FALSE)
```

Arguments

df a data frame

na.rm logical, remove NA values

log logical, use geometric mean instead of arithmetic mean

Value

A numeric vector

row_sd 29

row_sd	
--------	--

Compute the standard deviation by row

Description

Compute the standard deviation by row

Usage

```
row_sd(df)
```

Arguments

df a data frame

Value

A numeric vector

row_stoichio	Compute the stoichiometry of interaction using the method described
	in

Description

Compute the stoichiometry of interaction using the method described in ...

Usage

```
row_stoichio(df, idx_group_1, idx_group_2, idx_bait, Npep, log = TRUE,
   substract_ctrl = TRUE)
```

Arguments

df	a data frame	
idx_group_1	column indexes corresponding to the first group (bait background)	
idx_group_2	column indexes corresponding to the second group (ctrl background)	
idx_bait	row index for the bait protein	
Npep	numeric vector containing the number of theoretically observable peptides for each protein	
log	logical, use the geometric mean instead of the arithmetic mean	
substract_ctrl	substract_ctrl logical, substract ctrl intensities in the calculation of stoichiometries	

Value

A numeric vector of interaction stoichiometries

30 smooth_interactome

COM	ttest
I OW	LLESL

Perform a t-test comparison between two groups by row

Description

Perform a t-test comparison between two groups by row

Usage

```
row_ttest(df, idx_group_1, idx_group_2, log = TRUE)
```

Arguments

df a data frame

idx_group_1 column indexes corresponding to the first group
idx_group_2 column indexes corresponding to the second group
option to perform the t-test on log transformed data

Value

A data frame with columns 'p_val' and 'fold_change

smooth_interactome

 ${\it Smooth, using a moving average across conditions, selected variables of an {\tt InteRactome}}$

Description

Smooth, using a moving average across conditions, selected variables of an InteRactome

Usage

```
smooth_interactome(res, n = 1, order_conditions = NULL,
  var_smooth = c("fold_change", "p_val"))
```

Arguments

res an InteRactome

n integer, radius of the moving avergae (number of points extending on each side

of the center point on which the average is computed)

order_conditions

a numeric vector ordering conditions in res\$conditions

var_smooth variables on which the moving average will be computed

Value

an smoothed InteRactome

summary_table 31

summary_table

Create a summary table for an InteRactome

Description

Create a summary table for an InteRactome

Usage

```
summary_table(res, add_columns = names(res))
```

Arguments

res an InteRactome

add_columns names of the variables to display in the summary table

Value

a data.frame

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