# Package 'InteRact'

July 4, 2018

Title Analysis of Affinity Purification data
Version 0.1.0
<b>Date</b> 2018-02-21
Author Guillaume Voisinne
Maintainer Guillaume Voisinne <voisinne@ciml.univ-mrs.fr></voisinne@ciml.univ-mrs.fr>
<b>Description</b> This package contains useful functions to analyse affinity purification data
Imports dplyr, ggplot2, ggrepel, stringr, Hmisc, igraph, networkD3, ggsignif, PSICQUIC
LazyData TRUE
License file LICENSE
RoxygenNote 6.0.1
<b>Depends</b> R (>= 2.10)
Suggests testthat
LinkingTo Rcpp
Dinking IV Repp
R topics documented:
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

2 add\_GO\_data

discretize_values	. 10
dot_plot	. 10
estimate_Npep	
filter_conditions	. 11
filter_Proteins	
geom_mean	
get_annotations	. 13
get_PPI_from_BioGRID	. 13
get_PPI_from_HPRD	. 14
get_PPI_from_psicquic	. 14
global_analysis	. 15
identify_conditions	
identify_interactors	. 16
InteRact	. 17
mean_analysis	. 18
merge_conditions	. 19
merge_duplicate_groups	. 19
merge_proteome	
moving_average	. 20
order_interactome	
plot_2D_stoichio	
plot_annotation_results	
plot_comparison	
plot_correlation_network	
plot_per_condition	
plot_QC	
plot_stoichio	
plot_volcanos	
preprocess_data	
rescale_median	
row_mean	
row_sd	
row_stoichio	
row_ttest	
smooth_interactome	
summary_table	. 30
	21
	31

add\_GO\_data

Add GO annotations

### Description

Add GO annotations corresponding to a set of protein identifiers

### Usage

Index

```
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)
```

4 analyse\_interactome

#### **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

6 append\_FDR

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

10 dot\_plot

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

12 geom\_mean

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 proteomics data
--------------------------------------

### **Description**

This package implements several functions to analyze Affinity Purification 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**

1 8	guinents	
	df	A dataframe containing protein intensities. By default, protein intensity column names start by "Intensity." (use parameter Column_intensity_pattern to change)
	${\tt updateProgress}$	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 condition
	substract_ctrl	logical, substract ctrl intensities in the calculation of stoichiometries
	preprocess_df	list obtained by the function preprocess_data()
		$additionnal\ parameters\ passed\ to\ functions\ preprocess\_data()\ and\ identify\_conditions().$

### **Details**

By default, it is configured to work with proteinGroups.txt files generated by MaxQuant

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

### Value

```
a object 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.
```

18 mean\_analysis

```
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.
```

#### Author(s)

Guillaume Voisinne

#### **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, annot)</pre>
#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 InteRactom
--------------------------

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

22 plot\_comparison

```
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 = Interactome$conditions,
  ref_condition = Interactome$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

 $test.args \hspace{1.5cm} arguments \hspace{0.1cm} passed \hspace{0.1cm} to \hspace{0.1cm} function \hspace{0.1cm} test \hspace{0.1cm}$ 

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,
   ...)
```

rescale\_median 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

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\_sd

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

logical, use geometric mean instead of arithmetic mean

### Value

A numeric vector

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 29

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	logical, substract ctrl intensities in the calculation of stoichiometries

### Value

A numeric vector of interaction stoichiometries

row_ttest	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
log	option to perform the t-test on log transformed data

### Value

A data frame with columns 'p\_val' and 'fold\_change

30 summary\_table

smooth\_interactome

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

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

## **Index**

```
add_GO_data, 2
add_Hallmark_data, 3
add_KEGG_data, 3
analyse_interactome, 4
annotation_enrichment_analysis, 5
append_annotations, 6
append_FDR, 6
append_PPI, 7
average_technical_replicates, 7
compute_correlations, 8
compute_FDR_from_asymmetry, 8
{\tt create\_summary\_table\_PPI, 9}
discretize_values, 10
dot_plot, 10
estimate_Npep, 11
filter_conditions, 11
filter_Proteins, 12
geom_mean, 12
get_annotations, 13
get_PPI_from_BioGRID, 13
get_PPI_from_HPRD, 14
get_PPI_from_psicquic, 14
global_analysis, 15
{\tt identify\_conditions}, 15
identify_interactors, 16
InteRact, 17
mean_analysis, 18
merge_conditions, 19
merge_duplicate_groups, 19
merge_proteome, 20
moving_average, 20
order_interactome, 21
plot_2D_stoichio, 21
plot_annotation_results, 22
plot_comparison, 22
plot_correlation_network, 23
```

plot\_per\_condition, 24 plot\_QC, 25 plot\_stoichio, 25 plot\_volcanos, 26 preprocess\_data, 26 rescale\_median, 27 row\_mean, 28 row\_sd, 28 row\_stoichio, 29 row\_ttest, 29 smooth\_interactome, 30 summary\_table, 30