

Package ‘MSstatsBioNet’

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Type Package

Title Network Analysis for MS-based Proteomics Experiments

Version 1.1.3

Description A set of tools for network analysis using mass spectrometry-based proteomics data and network databases. The package takes as input the output of MSstats differential abundance analysis and provides functions to perform enrichment analysis and visualization in the context of prior knowledge from past literature. Notably, this package integrates with INDRA, which is a database of biological networks extracted from the literature using text mining techniques.

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Depends R (>= 4.4.0), MSstats

Imports RCy3, httr, jsonlite, r2r, tidyr, MASS

Suggests data.table, BiocStyle, knitr, rmarkdown, testthat (>= 3.0.0), mockery, MSstatsConvert

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URL <http://msstats.org>, <https://vitek-lab.github.io/MSstatsBioNet/>

BugReports <https://groups.google.com/forum/#!forum/msstats>

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Contents

.populateHgncIdsInDataFrame	2
.populateHgncNamesInDataFrame	2
.populateKinaseInfoInDataFrame	3
.populatePhosphataseInfoInDataFrame	3
.populateTranscriptionFactorInfoInDataFrame	4
.populateUniprotIdsInDataFrame	4
.validateAnnotateProteinInfoFromIndraInput	5
annotateProteinInfoFromIndra	5
getPathwaysFromIndra	6
getSubnetworkFromIndra	7
visualizeNetworks	8
Index	10

.populateHgncIdsInDataFrame	
<i>Populate HGNC IDs in Data Frame</i>	

Description

This function populates the HGNC IDs in the data frame based on the Uniprot IDs.

Usage

```
.populateHgncIdsInDataFrame(df)
```

Arguments

df A data frame containing protein information.

Value

A data frame with populated HGNC IDs.

.populateHgncNamesInDataFrame	
<i>Populate HGNC Names in Data Frame</i>	

Description

This function populates the HGNC names in the data frame based on the HGNC IDs.

Usage

```
.populateHgncNamesInDataFrame(df)
```

Arguments

df A data frame containing protein information.

Value

A data frame with populated HGNC names.

```
.populateKinaseInfoInDataFrame
```

Populate Kinase Info in Data Frame

Description

This function populates the kinase information in the data frame based on the HGNC names.

Usage

```
.populateKinaseInfoInDataFrame(df)
```

Arguments

df A data frame containing protein information.

Value

A data frame with populated kinase information.

```
.populatePhosphataseInfoInDataFrame
```

Populate Phosphatase Info in Data Frame

Description

This function populates the phosphatase information in the data frame based on the HGNC names.

Usage

```
.populatePhosphataseInfoInDataFrame(df)
```

Arguments

df A data frame containing protein information.

Value

A data frame with populated phosphatase information.

`.populateTranscriptionFactorInfoInDataFrame`*Populate Transcription Factor Info in Data Frame*

Description

This function populates the transcription factor information in the data frame based on the HGNC names.

Usage

```
.populateTranscriptionFactorInfoInDataFrame(df)
```

Arguments

`df` A data frame containing protein information.

Value

A data frame with populated transcription factor information.

`.populateUniprotIdsInDataFrame`*Populate Uniprot IDs in Data Frame*

Description

This function populates the Uniprot IDs in the data frame based on the protein ID type.

Usage

```
.populateUniprotIdsInDataFrame(df, proteinIdType)
```

Arguments

`df` A data frame containing protein information.

`proteinIdType` A character string specifying the type of protein ID. It can be either "Uniprot" or "Uniprot_Mnemonic".

Value

A data frame with populated Uniprot IDs.

`.validateAnnotateProteinInfoFromIndraInput`*Validate Annotate Protein Info Input*

Description

This function validates the input data frame for the `annotateProteinInfoFromIndra` function.

Usage

```
.validateAnnotateProteinInfoFromIndraInput(df)
```

Arguments

`df` A data frame containing protein information.

Value

None. Throws an error if validation fails.

`annotateProteinInfoFromIndra`*Annotate Protein Information from Indra*

Description

This function annotates a data frame with protein information from Indra.

Usage

```
annotateProteinInfoFromIndra(df, proteinIdType)
```

Arguments

`df` output of `groupComparison` function's `comparisonResult` table, which contains a list of proteins and their corresponding p-values, logFCs, along with additional HGNC ID and HGNC name columns

`proteinIdType` A character string specifying the type of protein ID. It can be either "Uniprot" or "Uniprot_Mnemonic".

Value

A data frame with the following columns:

Protein Character. The original protein identifier.

UniprotID Character. The Uniprot ID of the protein.

HgncID Character. The HGNC ID of the protein.

HgncName Character. The HGNC name of the protein.

IsTranscriptionFactor Logical. Indicates if the protein is a transcription factor.

IsKinase Logical. Indicates if the protein is a kinase.

IsPhosphatase Logical. Indicates if the protein is a phosphatase.

Examples

```
df <- data.frame(Protein = c("CLH1_HUMAN"))
annotated_df <- annotateProteinInfoFromIndra(df, "Uniprot_Mnemonic")
head(annotated_df)
```

getPathwaysFromIndra	<i>Get pathways ranked on relevance from INDRA DB</i>
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Description

Get pathways ranked on relevance from INDRA DB

Usage

```
getPathwaysFromIndra(
  annotated_df,
  main_target = "MEN1_HUMAN",
  target_type = "Protein"
)
```

Arguments

annotated_df	output of groupComparison function's comparisonResult table, which contains a list of proteins and their corresponding p-values, logFCs, along with additional HGNC ID and HGNC name columns
main_target	A main target, e.g. main target of a drug or protein of particular interest
target_type	One of either 'Protein' or 'Drug'. Default is 'Protein'

Value

df of pathways

Examples

```
annotated_df <- data.table::fread(system.file(
  "extdata/groupComparisonModel.csv",
  package = "MSstatsBioNet"
))
pathways <- getPathwaysFromIndra(annotated_df, "P05067")
head(pathways)
```

getSubnetworkFromIndra

Get subnetwork from INDRA database

Description

Using differential abundance results from MSstats, this function retrieves a subnetwork of protein interactions from INDRA database.

Usage

```
getSubnetworkFromIndra(
  input,
  protein_level_data = NULL,
  pvalueCutoff = NULL,
  statement_types = c("IncreaseAmount", "DecreaseAmount"),
  paper_count_cutoff = 1,
  evidence_count_cutoff = 1,
  correlation_cutoff = 0.3,
  sources_filter = NULL
)
```

Arguments

input	output of groupComparison function's comparisonResult table, which contains a list of proteins and their corresponding p-values, logFCs, along with additional HGNC ID and HGNC name columns
protein_level_data	output of the dataProcess function's ProteinLevelData table, which contains a list of proteins and their corresponding abundances. Used for annotating correlation information and applying correlation cutoffs.
pvalueCutoff	p-value cutoff for filtering. Default is NULL, i.e. no filtering
statement_types	list of interaction types to filter on. Equivalent to statement type in INDRA. Default is c("IncreaseAmount", "DecreaseAmount").
paper_count_cutoff	number of papers to filter on. Default is 1.
evidence_count_cutoff	number of evidence to filter on for each paper. E.g. A paper may have 5 sentences describing the same interaction vs 1 sentence. Default is 1.
correlation_cutoff	if protein_level_abundance is not NULL, apply a cutoff for edges with correlation less than a specified cutoff. Default is 0.3
sources_filter	filtering only on specific sources. Default is no filter, i.e. NULL. Otherwise, should be a list, e.g. c('reach', 'medscan').

Value

list of 2 data.frames, nodes and edges

Examples

```
input <- data.table::fread(system.file(
  "extdata/groupComparisonModel.csv",
  package = "MSstatsBioNet"
))
subnetwork <- getSubnetworkFromIndra(input)
head(subnetwork$nodes)
head(subnetwork$edges)
```

visualizeNetworks	<i>Create visualization of network</i>
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Description

Use results from INDRA to generate a visualization of the a network on Cytoscape Desktop. Note that the Cytoscape Desktop app must be open for this function to work.

Usage

```
visualizeNetworks(
  nodes,
  edges,
  pvalueCutoff = 0.05,
  logfcCutoff = 0.5,
  node_label_column = "id",
  main_targets = c()
)
```

Arguments

nodes	dataframe of nodes consisting of columns id (character), pvalue (number), logFC (number)
edges	dataframe of edges consisting of columns source (character), target (character), interaction (character), evidenceCount (number), evidenceLink (character)
pvalueCutoff	p-value cutoff for coloring significant proteins. Default is 0.05
logfcCutoff	log fold change cutoff for coloring significant proteins. Default is 0.5
node_label_column	The column of the nodes dataframe to use as the node label. Default is "id". "hgncName" can be used for gene name.
main_targets	character vector of main targets to stand-out with a different node shape. Default is an empty vector c(). IDs of main targets should match the column used by the node_label_column parameter.

Value

cytoscape visualization of subnetwork

Examples

```
input <- data.table::fread(system.file(
  "extdata/groupComparisonModel.csv",
  package = "MSstatsBioNet"
))
subnetwork <- getSubnetworkFromIndra(input)
visualizeNetworks(subnetwork$nodes, subnetwork$edges)
```

Index

.populateHgncIdsInDataFrame, [2](#)
.populateHgncNamesInDataFrame, [2](#)
.populateKinaseInfoInDataFrame, [3](#)
.populatePhosphataseInfoInDataFrame, [3](#)
.populateTranscriptionFactorInfoInDataFrame,
 [4](#)
.populateUniprotIdsInDataFrame, [4](#)
.validateAnnotateProteinInfoFromIndraInput,
 [5](#)

annotateProteinInfoFromIndra, [5](#)

dataProcess, [7](#)

getPathwaysFromIndra, [6](#)
getSubnetworkFromIndra, [7](#)
groupComparison, [5–7](#)

visualizeNetworks, [8](#)