Package 'DrugSim2DR'

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Type Package

Title Predict Drug Functional Similarity to Drug Repurposing

Version 0.1.1

Maintainer Junwei Han <hanjunwei1981@163.com>

Description A systematic biology tool was developed to repurpose drugs via a drug-drug functional similarity network. 'DrugSim2DR' first predict drug-drug functional similarity in the context of specific disease, and then using the similarity constructed a weighted drug similarity network. Finally, it used a network propagation algorithm on the network to identify drugs with significant target abnormalities as candidate drugs.

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Encoding UTF-8

LazyData true

RoxygenNote 7.2.1

Imports igraph, stats, pheatmap, ChemmineR, rvest, base, sp, tidyr, reshape2, fastmatch

Suggests knitr, rmarkdown

VignetteBuilder knitr

Depends R (>= 3.6)

NeedsCompilation no

Author Junwei Han [aut, cre, cph],
Ji Li [aut],
Jiashuo Wu [aut]

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Contents

`CalDEscore` *CalDEscore*

Description

Function "CalDEscore" uses gene expression to calculate differential expression level.

Usage

```
CalDEscore(exp, Label)
```

Arguments

`exp`	A gene expression profile of interest (rows are genes, columns are samples).
`Label`	A character vector consist of "0" and "1" which represent sample class in the gene expression profile. "0" means normal sample and "1" means disease sample.

Value

A matrix with one column of zscore.

Examples

```
# Obtain the example data
GEP<-Gettest("GEP")
label<-Gettest("label")
# Run the function
DEscore<-CalDEscore(GEP,label)
```

`datasummary` *datasummary: Custom Data Summaries*

Description

Easily generate custom data frame summaries

Author(s)

Maintainer: Junwei Han <hanjunwei1981@163.com> [copyright holder]

Authors:

- Ji Li
- Jiashuo Wu

`DrugReposition` *DrugReposition*

Description

The function "DrugReposition" is used in drug repositioning by calculating the eigenvector centrality of drugs.

Usage

```
DrugReposition(DE,nperm = 1000,r = 0.9,p = 10^-10)
```

Arguments

`DE`	A matrix with one column of zscore.
`nperm`	Number of random permutations (default: 1000).
`r`	Restart the probability of the random-walk algorithm (default: 0.9).
`p`	For each node, if the difference in centrality score between iterations changes less than this value, the algorithm considers the calculation complete (default: 10^-10).

Value

A dataframe with seven columns those are drugbankid, centralscore, p.value,fdr,number of targets, drug targets,drugname.

Examples

```
library("igraph")
# Obtain the example data
GEP<-Gettest("GEP")
label<-Gettest("label")
# Run the function
DEscore<-CalDEscore(GEP,label)
# Run the function
drug_centrality<-DrugReposition(DE=DEscore,nperm = 1000,r = 0.9,p = 10^-10)
```

DrugSimscore *DrugSimscore*

Description

The function "DrugSimscore" is used in calculating the drug functional similarity score.

Usage

```
DrugSimscore(DE,nperm = 0)
```

Arguments

DE	A matrix with one column of zscore.
nperm	Number of random permutations (default: 0).

Value

A dataframe with four columns those are drug1, drug2, drug1 name, drug2 name, functional similarity score and FDR.

Examples

```
# Obtain the example data
GEP<-Gettest("GEP")
label<-Gettest("label")
# Run the function
DEscore<-CalDEscore(GEP,label)
# Run the function
drug_drug<-DrugSimscore(DE=DEscore,nperm = 0)
```

Gettest *Gettest*

Description

Get the example data

Usage

```
Gettest(exampleData)
```

Arguments

exampleData	A character,should be one of"Jaccard","commongenes","GO_MF","Drugs","Drugbankid_CID","drugnan

Value

data

myenv *An environment variable which includes some example data*

Description

An environment variable which includes some example data. Jaccard:A matrix of Jaccard score between drugs and GOMF. commongenes:A matrix consisting of genes shared by drug targets and GOMF. GO_MF:GO terms of molecular functions. Drugs:Drugs and corresponding targets. GEP:An example gene expression profile. label:A vector representing the label of the sample of GEP, where "1" is the disease sample and "0" is the normal sample. Drugbankid_CID:A dataframe including three columns which are drugbankid, ChembleID, and drugname.

Usage

```
myenv
```

Format

An environment variable

plotDruglink *plotDruglink*

Description

The function "plotDruglink" is used to plot a bipartite network of drugs and shared molecular functions.

Usage

```
plotDruglink(drug1,drug2,i = 5,color_MF = "#43AAEF",color_drug = "#F7525B",
layout_type = "circle")
```

Arguments

drug1	The drugbank ID of drug1.
drug2	The drugbank ID of drug2.
i	Specifies the number of outputs molecular functions, which is 5 by default.
color_MF	Defines the color of MF nodes in the network.
color_drug	Defines the color of drug nodes in the network.
layout_type	layout_type used to set the appropriate arrangement, there is an option to choose from "circle","dh",and "sugiyama".

Value

A bipartite network of drugs and shared molecular functions.

Examples

```
# Set drug1
drug1<-"DB02721"
# Set drug2
drug2<-"DB01213"
# Run the function
library(igraph)
plotDruglink(drug1,drug2,i = 5)
```

plotDrugstructure *plotDrugstructure*

Description

The function "plotDrugstructure" can plot the chemical structure of a drug.

Usage

```
plotDrugstructure(drugid = "")
```

Arguments

drugid	A drugbank ID.

Value

A chemical structure of specific drug

Examples

```
# Load depend package
library(ChemmineR)
library(rvest)
# Obtain molecular formula and visualize it.
plotDrugstructure(drugid ="DB00780")
```

plotTargetheatmap *plotTargetheatmap*

Description

The function "plotTargetheatmap" is used to plot a heat map of drug targets expression.

Usage

```
plotTargetheatmap(drugid,ExpData,label,significance=FALSE,
cluster.rows=FALSE,cluster.cols=FALSE,bk=c(-2.4,2.3),show.rownames=TRUE,
show.colnames=FALSE,ann_colors=c("#FFAA2C","#2CBADA"),col=c("#2A95FF","#FF1C1C"))
```

Arguments

drugid	The drugbank ID of a drug.
ExpData	A gene expression profile of interest (rows are genes, columns are samples).
label	A character vector consists of "0" and "1" which represent sample class in the gene expression profile. "0" means normal sample and "1" means disease sample.
significance	This parameter controls whether the p-value of differential expression is displayed.
cluster.rows	Logical value that represents whether row clustering is used.
cluster.cols	Logical value that represents whether col clustering is used.
bk	This parameter adjusts the range of values displayed by the color bar.
show.rownames	This parameter controls whether row names are displayed.
show.colnames	This parameter controls whether column names are displayed.
ann_colors	Vector of colors used to define groups.
col	Vector of colors used in the heatmap.

Value

A heat map of drug targets expression.

Examples

```
# Obtain the example data
GEP<-Gettest("GEP")
label<-Gettest("label")
# Run the function
plotTargetheatmap("DB00780",GEP,label)
```

Index