

Package ‘DrugSim2DR’

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Type Package

Title Predict Drug Functional Similarity to Drug Repurposing

Version 0.1.0

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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

Suggests knitr, rmarkdown

VignetteBuilder knitr

Depends R (>= 3.6)

NeedsCompilation no

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 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)

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 DrugReposition

DrugReposition

Description

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

Usage

```
DrugReposition(DE,nperm = 100,r = 0.9,p = 10^-10)
```

Arguments

DE	A matrix with one column of zscore.
nperm	Number of random permutations (default: 100).
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

```
# 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 = 100,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", "drugname"

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	<i>plotDruglink</i>
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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

<code>drugid</code>	The drugbank ID of a drug.
<code>ExpData</code>	A gene expression profile of interest (rows are genes, columns are samples).
<code>label</code>	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.
<code>significance</code>	This parameter controls whether the p-value of differential expression is displayed.
<code>cluster.rows</code>	Logical value that represents whether row clustering is used.
<code>cluster.cols</code>	Logical value that represents whether col clustering is used.
<code>bk</code>	This parameter adjusts the range of values displayed by the color bar.
<code>show.rownames</code>	This parameter controls whether row names are displayed.
<code>show.colnames</code>	This parameter controls whether column names are displayed.
<code>ann_colors</code>	Vector of colors used to define groups.
<code>col</code>	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)
```


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