Package 'PriorCD'

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Type Package

Title Prioritizing Cancer Drugs for Interested Cancer

Version 0.1.0

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Description

Prioritize candidate cancer drugs for drug repositioning based on the random walk with restart algorithm in a drug-drug functional similarity network. 1) We firstly constructed a drug-drug functional similarity network by integrating pathway activity and drug activity derived from the NCI-60 cancer cell lines. 2) Secondly, we calculated drug repurposing score according to a set of approved therapeutic drugs of interested cancer based on the random walk with restart algorithm in the drug-drug functional similarity network. 3) Finally, the permutation test was used to calculate the statistical significance level for the drug repurposing score.

License GPL (>= 2)

Encoding UTF-8

LazyData true

RoxygenNote 6.1.1

Imports igraph, dplyr, ROCR, visNetwork

Suggests knitr, rmarkdown

Depends R (>= 2.10)

VignetteBuilder knitr

NeedsCompilation no

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R topics documented:

`PriorCD-package` *Prioritizing cancer drugs for interested cancer*

Description

This package implements methods to predict priorities of therapeutic drugs against interested cancer by combining drug functional similarity network and global network propagation algorithm. Besides, users can validate the prioritizing results and visualize the network structure of the resultant drugs.

`drsim` *drsim*

Description

This function is used to construct a binary adjacency matrix of drug similarity where 1 means strong similarity and 0 means weak similarity.

Usage

```
drsim(r.mat, p.mat, top = 0.005, r.thres = 0.7, p.thres = 0.01)
```

Arguments

`r.mat`	The input matrix of drug correlations.
`p.mat`	The input matrix of probability values(p-value) of drug correlations.
`top`	A value to measure drug similarity. It's a threshold of correlation, top=0.005(default) means that top 0.005 of drugs for each row are considered as strong similarity.
`r.thres`	A value to measure drug similarity. It's a threshold of correlation, r.thres=0.7(default) means that the similarity between drugs are strong when r greater than 0.7.
`p.thres`	A value to measure the significance level of drug similarity. It's a threshold of probability values, p.thres=0.01(default) means that the similarity between drugs are significant when p less than 0.01.

Value

A binary adjacency matrix of drug similarity.

Examples

```
r <- getData("drug.r")
fdr <- getData("drug.fdr")
m <- drsim(r, fdr, top = 0.5)
```

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envData *The variables in the environment include an example profile, a edge-list of our drug simiarity network, comprehensive drug information, restart drug set of breast cancer, candidate drugs of breast cancer, fdr of drug similarity network, correlation between drugs, mRNA and microRNA pathway activity profiles we've enriched.*

Description

Drug repurposing has become the focus of experts in drug development. In PriorCD, pathway activities and drug activities are combine to construct drug functional similarity network, and on which a global network propagation algorithm is applied. First, drug functional similarity network is constructed by the correlation and fdr of drug pairs. Then a global netwokr propagation (RWR) is performed on this network to prioritize candidates. Finally, ROC and network structure of the result can be browsed in PriorCD by getROC and getDDN functions.

Format

An environment variable

Details

The environment variable includes the variable `drug.edgelist`, `drug.info`,`brc_candidates`,`breast_cancer`,`drug.fdr`,`dr`

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getData *getData*

Description

This function is used to get example data.

Usage

```
getData(exampleData)
```

Arguments

exampleData	String. These example data are included: mRNA_path, microRNA_path, drug.ic50, drug.r, drug.fdr, drug.info, drug.edgelist, breast_cancer and brc_candidates.

getDDN *getDDN*

Description

This function is used to generate drug drug similarity network.

Usage

```
getDDN(drug.el, r.set, candidates, file = "network.html")
```

Arguments

drug.el	A edge list of drugs, which is a two-column matrix, each row defines one edge. Numbers in the edge list represent NSC-ID of drugs.
r.set	A set of drugs that you used to prioritize candidates.
candidates	A set of drugs that have been prioritized.
file	file = "network.html"(default). File name and path where to save the HTML web page. Currently only .html formats are supported.

Value

A HTML web page within drug drug similarity network

Examples

```
e <- getData("drug.edgelist")
brc <- getData("breast_cancer")
candidates <- getData("brc_candidates")
getDDN(e, brc, candidates)
```

getROC *getROC*

Description

This function is used to plot ROC.

Usage

```
getROC(drug.el, p0, gamma = 0.7, filename = "ROC.pdf")
```

Arguments

drug.el	A edge list of drugs, which is a two-column matrix, each row defines one edge. Numbers in the edge list represent NSC-ID of drugs.
p0	A vector of approved drugs' NSC-ID of interested cancer.
gamma	gamma=0.7(default). A probability of losing when doing Random Walk. On the contray, there is a probability of 1-gamma left to itself. The range of this value is (0, 1).
filename	filename = "ROC.pdf"(default). File name and path where to save the PDF. Filetype is decided by the extension in the path. Currently only .pdf formats are supported.

Value

ROC

Examples

```
e <- getData("drug.edgelist")
brc <- getData("breast_cancer")
getROC(e, brc)
```

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prior *prior*

Description

This function is used to generate drug prioritizing result.

Usage

```
prior(drug.el, p0, gamma = 0.7, times = 100)
```

Arguments

drug.el	A edge list of drugs, which is a two-column matrix, each row defines one edge. Numbers in the edge list represent NSC-ID of drugs.
p0	A vector of approved drugs' NSC-ID of interested cancer.
gamma	gamma = 0.7(default). A probability of losing when doing Random Walk. On the contray, there is a probability of 1-gamma left to itself. The range of this value is (0, 1).
times	times = 100(default). Loop times when getting p-values.

Value

Detailed information about drug prioritizing, which contain NSC-id, name, prioritizing score, p-value, FDR, status and MOA(mechanism of action) of drugs.

Examples

```
e <- getData("drug.edgelist")
brc <- getData("breast_cancer")
result <- prior(e, brc,time=20)
```

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