Package ‘SubtypeDrug’

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Type Package

Title Prioritization of Candidate Cancer Subtype Specific Drugs

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Imports BiocGenerics,GSVA,grDevices,graphics,igraph,parallel,pheatmap,rvest,stats,xml2,ChemmineR

Suggests knitr, rmarkdown

VignetteBuilder knitr

NeedsCompilation no

Repository CRAN

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AccumulateNormal

SubtypeDrug internal function

Description
Infering patient-specific subpathway activity profiles.

Usage
AccumulateNormal(x_matrix, control_index)

Arguments
x_matrix A subpathway activity profile. rows are subpathways, columns are samples.
control_index A vector. In the sample of the subpathway activity profile, the position of control samples.

Details
AccumulateNormal
Description

Calculate subpathway enrichment score.

Usage

CalculateSES(labels.list, correl.vector = NULL)

Arguments

labels.list A vector of 0 and 1.
correl.vector A vector. The weight value used to calculate the enrichment score.

Examples

x<-matrix(c(1:10),ncol = 5)
x1<-AccumulateNormal(x,c(3,5))

x<-CalculateSES(sample(c(0,1),10,replace = TRUE),c(1:10))
Colork

Description
This variable stores the color data required by the program.

Usage
Colork

Format
A vector containing 73 values.

Examples
data(Colork)

Disease_drugs

Description
The simulated result data of only two sample types is generated by the functional PrioSubtypeDrug.

Usage
Disease_drugs

Format
A list containing 8 variables. The variables are as follows:

- Cacner Results table for cacner
- SubpathwayMatrix Subpathway activity matrix
- SampleInformation Cancer sample phenotypic information
- Parameter Parameter of the function PrioSubtypeDrug

Examples
# data(Disease_drugs)
Drugs_CID

Correspondence table of drug label and drug ID in PubCham database

Description
A data frame for the drug and its corresponding PubCham database ID.

Usage
Drugs_CID

Format
A dataframe with drug label and CID. The variables are as follows:

- Drugs Drug label
- CID Drug ID in PubCham database

Examples
data(Drugs_CID)

Geneexp
Simulated gene expression data

Description
Simulated normalized gene expression profile data.

Usage
Geneexp

Format
A matrix with 3000 genes and 40 samples.

Examples
data(Geneexp)
GeneexpT  

*Gene expression data for testing*

Description
Simulated normalized gene expression profile data.

Usage
GeneexpT

Format
A matrix with 40 samples.

Examples

data(GeneexpT)

getDrugMatrix  

*SubtypeDrug internal function*

Description
Obtaining drug-disease reverse association score matrix.

Usage
getDrugMatrix(spw_matrix, drug_target_data, weighted.score)

Arguments

- `spw_matrix`: A subpathway activity profile. rows are subpathways, columns are samples.
- `drug_target_data`: A list. A list stores a collection of drug up- and down-regulated subpathways.
- `weighted.score`: A binary value of 0 or 1. If the ‘weighted.score’ = 1, the drug reverse association score will be weighted by the subpathway activity.

Details
getDrugMatrix

Value
A matrix.
### Description

According to the parameters set by the user, the up-regulatory and down-regulatory subpathway data of drug is obtained.

### Usage

```r
getDrugSpw(
  drug_target_data,
  spw_matrix_rnames,
  drug.P.value.threshold,
  drug.min.sz,
  drug.max.sz
)
```

### Arguments

- **drug_target_data**
  A list. A list stores a collection of drug up- and down-regulated subpathways.

- **spw_matrix_rnames**
  A vector. A vector consisting of row names of subpathway activity profile.

- **drug.P.value.threshold**
  A value. According to the threshold of the significant P value set by parameter `drug.p.val.threshold`, the drug up-regulation and down-regulatory subpathways were screened.

- **drug.min.sz**
  A numeric. The drug regulated subpathways intersects with the subpathways in the subpathway activity profile. Then drugs with less than `drug.spw.min.sz` up- or down-regulated subpathways are removed.

- **drug.max.sz**
  A numeric. Similar to parameter `drug.spw.min.sz`, drugs with more than `drug.spw.max.sz` up- or down-regulated subpathways are removed.
getDrugStructure

Details

getDrugSpw

Value

a list.

Author(s)

Xudong Han, Junwei Han, Chonghui Liu

Examples

require(GSVA)
Geneexp<-get("Geneexp")
UserGS<-get("UserGS")
UserDS<-get("UserDS")
spw_matrix<-gsva(Geneexp,UserGS,verbose=FALSE)
x<-getDrugSpw(UserDS,row.names(spw_matrix),0.05,1,100)

getDrugStructure  Get drug chemical structure diagram data

Description

‘getDrugStructure()’ outputs the chemical structure graph data of the drug or compound based on the input drug label by the user. The results can be visualized by the ‘plot’ function.

Usage

getDrugStructure(drug.label = "", main = "", sub = "")

Arguments

drug.label A character string of drug label to determine which drug to use for visualization.
main An overall title for the chemical structure graph.
sub A sub title for the chemical structure graph.

Details

getDrugStructure

Value

A sdfset object.
isPackageLoaded

Author(s)
Xudong Han, Junwei Han, Chonghui Liu

Examples

```r
require(rvest)
require(ChemmineR)
# Plot the chemical structure of drug pirenperone.
# Chem_str<-getDrugStructure(drug.label="pirenperone.")
# plot(Chem_str)
```

Description
Determine if the package is loaded. If the package is not loaded, the program will prompt the user.

Usage

```r
isPackageLoaded(name)
```

Arguments

name A string. The name of the R package which determines whether it is loaded.

Details
isPackageLoaded

Value
A string, TRUE or FALSE.

Author(s)
Xudong Han, Junwei Han, Chonghui Liu

Examples

```r
isPackageLoaded("pheatmap")
```
plotDScoreHeatmap

Plot a heat map of the normalized drug-disease reverse association scores for cancer samples

Description

According to the parameter setting, the function `plotDScoreHeatmap()` displays the heat map of the normalized drug-disease reverse association score for the significant drugs.

Usage

```r
plotDScoreHeatmap(
    data,
    subtype.label = "all",
    SDS = "all",
    E_Pvalue.th = 1,
    E_FDR.th = 0.05,
    S_Pvalue.th = 1,
    S_FDR.th = 0.001,
    show.rownames = TRUE,
    show.colnames = FALSE,
    color = colorRampPalette(c("#0A8D0A", "#F8F0EB", "red"))(190),
    subtype_colors = NA,
    drug_colors = NA,
    border_color = "grey60",
    cellwidth = NA,
    cellheight = NA,
    fontsize = 10,
    fontsize.row = 10,
    fontsize.col = 10,
    scale = "row"
)
```

Arguments

data A list of result data generated by function `PrioSubtypeDrug()`.

subtype.label Character string indicates which sample of the cancer subtype was used to plot the heat map. If subtype.label = "all" (default), all cancer samples will be shown in the heat map.

SDS A string indicates that the range of SDS is used for the heat map. If SDS="all" (default), all cancer samples will be used. SDS="negative", only drugs with SDS<0 are used. SDS="positive", only drugs with SDS>0 are used.

E_Pvalue.th A numeric. A threshold is used to filter the drug effected P value (default: 1).

E_FDR.th A numeric. A threshold is used to filter the drug effected FDR (default: 0.05).

S_Pvalue.th A numeric. A threshold is used to filter the Subtype specific P value (default: 1).
plotDScoreHeatmap

S_FDR.th A numeric. A threshold is used to filter the Subtype specific P value (default: 0.001).
show.rownames Boolean specifying if row names are shown (default: TRUE).
show.colnames Boolean specifying if column names are shown (default: FALSE).
color Vector of colors used in heatmap.
subtype_colors Vector of colors is used to annotate the sample subtype. Its length should correspond to the number of sample subtypes.
drug_colors Vector of colors is used to label subtype-specific drugs.
border_color Color of cell borders on heatmap, use NA if no border should be drawn.
cellwidth Individual cell width in points. If left as NA, then the values depend on the size of plotting window.
cellheight Individual cell height in points. If left as NA, then the values depend on the size of plotting window.
fontsize Base fontsize for the plot (default: 10).
fontsize.row Fontsize for rownames (default: 10).
fontsize.col Fontsize for colnames (default: 10).
scale Character indicating if the values should be centered and scaled in either the row direction or the column direction, or none. Corresponding values are "row" (default), "column" and "none".

Details

plotDScoreHeatmap

Value

A heat map.

Author(s)

Xudong Han, Junwei Han, Chonghui Liu

Examples

require(pheatmap)
## Get the result data of PrioSubtypeDrug().
## The data is based on the simulated breast cancer subtype data.
Subtype_drugs<-get("Subtype_drugs")
## Heat map of all subtype-specific drugs.
#plotDScoreHeatmap(data=Subtype_drugs,E_Pvalue.th=0.05,
#                  S_Pvalue.th=0.05)
## Plot only Basal subtype-specific drugs.
plotDScoreHeatmap(Subtype_drugs,subtype.label="Basal",SDS="all",E_Pvalue.th=0.05,
                   E_FDR.t=1,S_Pvalue.th=0.05,S_FDR.th=1)
plotDSpwHeatmap

**Plot heat map of the drug regulated subpathway activity score**

**Description**

The `plotDSpwHeatmap()` function plots a heat map of the subpathways that are regulated by specified drug and have differential expression between specified cancer subtype and normal.

**Usage**

```r
plotDSpwHeatmap(
  data,
  drug.label = "",
  subtype.label = "",
  show.rownames = TRUE,
  show.colnames = TRUE,
  color = NA,
  phen_colors = NA,
  border_color = "grey60",
  cellwidth = NA,
  cellheight = NA,
  fontsize = 10,
  fontsize.row = 10,
  fontsize.col = 10,
  scale = "row"
)
```

**Arguments**

<table>
<thead>
<tr>
<th>Argument</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>data</td>
<td>A list of result data generated by function ‘PrioSubtypeDrug()’.</td>
</tr>
<tr>
<td>drug.label</td>
<td>A character string of drug labels to determine which drug to use for visualization.</td>
</tr>
<tr>
<td>subtype.label</td>
<td>Character string indicates which sample of the cancer subtype was used to plot the heat map.</td>
</tr>
<tr>
<td>show.rownames</td>
<td>Boolean specifying if row names are be shown.</td>
</tr>
<tr>
<td>show.colnames</td>
<td>Boolean specifying if column names are be shown.</td>
</tr>
<tr>
<td>color</td>
<td>Vector of colors used in heatmap.</td>
</tr>
<tr>
<td>phen_colors</td>
<td>Vector of colors is used to annotate the sample subtype and control sample. It should be assigned two colors.</td>
</tr>
<tr>
<td>border_color</td>
<td>Color of cell borders on heatmap, use NA if no border should be drawn.</td>
</tr>
<tr>
<td>cellwidth</td>
<td>Individual cell width in points. If left as NA, then the values depend on the size of plotting window.</td>
</tr>
<tr>
<td>cellheight</td>
<td>Individual cell height in points. If left as NA, then the values depend on the size of plotting window.</td>
</tr>
</tbody>
</table>
plotGlobalGraph

**Description**

The `plotGlobalGraph()` identifies the drug label entered by the user, and plots an integrated diagram including box plot of the normalized drug-disease reverse association scores, null distribution curves of significant P-value, and heat map of cancer subtype sample distribution.

```
plotGlobalGraph

fontsize
Base fontsize for the plot (default: 10).

fontsize.row
Fontsize for rownames (default: 10).

fontsize.col
Fontsize for colnames (default: 10).

scale
Character indicating if the values should be centered and scaled in either the row direction or the column direction, or none. Corresponding values are "row", "column" and "none".

Details

plotDSpwHeatmap

Based on the input cancer subtype, the program draws a heat map of the drug regulated subpathway activity score. If the cancer subtype of input has subtype-specific drug score (SDS)<0, we can observe the drug upregulatory subpathway is lowly expressed in the cancer subtype samples and high in the normal samples; the drug downregulatory subpathway is highly expressed in the cancer subtype samples and low in the normal samples. This indicates that after the drug action, these subpathways activity is converted from the level of the cancer subtype into the level of normal. If the cancer subtype of input has subtype-specific drug score (SDS)>0, it is indicated that the drug action may promote the subpathway expression status of the cancer subtype.

Value

A heat map.

Author(s)

Xudong Han, Junwei Han, Chonghui Liu

Examples

```r
require(pheatmap)
## Get the result data of PrioSubtypeDrug().
## The data is based on the simulated breast cancer subtype data.
Subtype_drugs<-get("Subtype_drugs")
plotDSpwHeatmap(data=Subtype_drugs,drug.label="pirenperone(1.02e-05M)",subtype.label="Basal")
## Visualize the results of only two types of samples.
Disease_drugs<-get("Disease_drugs")
plotDSpwHeatmap(data=Disease_drugs,drug.label="W-13(1e-05M)",subtype.label="Cancer")
```
Usage

plotGlobalGraph(
  data,
  drug.label = "",
  overall.main = "",
  overall.cex.main = 1.5,
  cex.submap.axis = 1,
  cex.submap.lab = 1,
  cex.submap.main = 1,
  cex.submap.sub = 1,
  cex.legend = 1
)

Arguments

data A list of result data generated by function ‘PrioSubtypeDrug()’.
drug.label A character string of drug labels to determine which drug to use for visualization.
overall.main An overall title for the whole graph. If the user does not make any input, the title will display a drug label.
overall.cex.main The magnification to be used for overall.main (default: 1.5).
cex.submap.axis The magnification to be used for axis of each submap annotation relative to the current setting of cex.
cex.submap.lab The magnification to be used for x and y labels of each submap relative to the current setting of cex.
cex.submap.main The magnification to be used for main titles of each submap relative to the current setting of cex.
cex.submap.sub The magnification to be used for sub titles of each submap relative to the current setting of cex.
cex.legend fontsize of labels for legend.

Details

plotGlobalGraph

Value

A plot.

Author(s)

Xudong Han, Junwei Han, Chonghui Liu
Examples

## Get the result data of PrioSubtypeDrug().
## The data is based on the simulated breast cancer subtype data.
Subtype_drugs<-get("Subtype_drugs")
## Plot a global graph of the drug pirenperone(1.02e-05M).
plotGlobalGraph(data=Subtype_drugs,drug.label="pirenperone(1.02e-05M)")

plotSpwNetGraph

Polt a subpathway network graph

Description

Visualize a subpathway network graph.

Usage

plotSpwNetGraph(
  spwid,
  layout = NULL,
  margin = 0,
  vertex.label.cex = 0.6,
  vertex.label.font = 1,
  vertex.size = 8,
  vertex.size2 = 6,
  edge.arrow.size = 0.2,
  edge.label.cex = 0.6,
  vertex.label.color = "black",
  vertex.color = "#BFFFBF",
  vertex.frame.color = "dimgray",
  edge.color = "dimgray",
  edge.label.color = "dimgray",
  sub = NULL,
  main = NULL
)

Arguments

spwid  The subpathway id which the user wants to plot.
layout  A matrix of x-y coordinates with two dims. Determine the placement of the
         nodes for drawing a graph.
margin  A numeric. The value is usually between -0.5 and 0.5, which is able to zoom in
         or out a subpathway graph. The default is 0.
vertex.label.cex  A numeric vector of node label size.
vertex.label.font
A numeric vector of label font.

vertex.size
A numeric vector of Node size. See \texttt{plot.igraph}.

vertex.size2
A numeric vector of Node size.

edge.arrow.size
Edge arrow size. The default is 0.2.

edge.arrow.width
Edge arrow width. The default is 3.

edge.label.cex
Edge label size.

vertex.label.color
A vector of node label colors. The default is black.

vertex.color
A vector of node colors. The default is the KEGG node color.

vertex.frame.color
A vector of node frame color. The default is dimgray.

edge.color
A vector of edge color. The default is dimgray.

edge.label.color
A vector of edge label color. The default is dimgray.

sub
A character string of subtitle.

main
A character string of main title.

Details

\texttt{plotSpwNetGraph}

The function \texttt{plotSpwNetGraph} is able to display a subpathway graph. The argument \texttt{layout} is used to determine the placement of the nodes for drawing a graph. The layouts provided in igraph include 'layout_as_star', 'layout_as_tree', 'layout_in_circle', 'layout_nicely', 'layout_on_grid', 'layout_on_sphere', 'layout_randomly', 'layout_with_dh', 'layout_with_fr', 'layout_with_gem', 'layout_with_graphopt', 'layout_with_kk', 'layout_with_lgl', 'layout_with_mds'. The 'layout_as_tree' generates a tree-like layout, so it is mainly for trees. The 'layout_randomly' places the nodes randomly. The 'layout_in_circle' places the nodes on a unit circle. Detailed information on the parameters can be found in \texttt{layout}.

Value

a plot

Author(s)

Xudong Han, Junwei Han, Chonghui Liu

Examples

```
require(igraph)
# plot network graph of the subpathway 00020_4.
plotSpwNetGraph(spwd="00020_4")
```
**PrioSubtypeDrug**

**Prioritization of candidate cancer subtype-specific drugs (PrioSubtypeDrug)**

---

**Description**

Integrating drug, gene, and subpathway data to identify drugs specific to cancer subtypes.

**Usage**

```r
PrioSubtypeDrug(
  expr,
  input.cls = "",
  control.label = "",
  subpathway.list,
  spw.min.sz = 10,
  spw.max.sz = Inf,
  spw.score.method = "gsva",
  kcdf = "Gaussian",
  drug.spw.data,
  drug.spw.p.val.th = 0.05,
  drug.spw.min.sz = 10,
  drug.spw.max.sz = Inf,
  weighted.drug.score = TRUE,
  nperm = 1000,
  parallel.sz = 1,
  E_FDR = 0.05,
  S_FDR = 0.001
)
```

**Arguments**

- **expr**
  - Matrix of gene expression values (rows are genes, columns are samples).
- **input.cls**
  - Input sample subtype class vector file in CLS format.
- **control.label**
  - In the CLS file of `input.cls`, the label of the control sample.
- **subpathway.list**
  - A list. The subpathway list data is mined from KEGG data and can be downloaded through the connection [https://github.com/hanjunwei-lab/SubtypeDrugData](https://github.com/hanjunwei-lab/SubtypeDrugData). The gene tags included in the subpathway list data should be consistent with those in the gene expression profile. The package ‘SubtypeDrugData’ provides two choices that include the Entrezid and Symbol tags of the gene. Users can also enter their own pathway or gene set list data.
- **spw.min.sz**
  - Removes subpathways that contain fewer genes than `spw.min.sz` (default: 10).
- **spw.max.sz**
  - Removes subpathways that contain more genes than `spw.max.sz` (default: Inf).
spw.score.method
Method to employ in the estimation of subpathway enrichment scores per sample. By default this is set to ‘gsva’ (Hänzelmann et al, 2013) and other options are ‘ssgsea’ (Barbie et al, 2009).

kcdf
Character string denoting the kernel to use during the non-parametric estimation of the cumulative distribution function of expression levels across samples when ‘spw.score.method=“gsva”‘. By default, ‘kcdf=“Gaussian”‘ which is suitable when input expression values are continuous, such as microarray fluorescent units in logarithmic scale, RNA-seq log-CPMs, log-RPKMs or log-TPMs. When input expression values are integer counts, such as those derived from RNA-seq experiments, then this argument should be set to ‘kcdf=“Poisson”‘.

drug.spw.data
A list data of drug regulation. The drug subpathway association data we constructed is stored in package ‘SubtypeDrugData’ and can be downloaded via connection https://github.com/hanjunwei-lab/SubtypeDrugData. If the input is user-defined drug regulation data, the data should be a list data with each drug as its element. Each drug also contains ‘Target_upregulation’ and ‘Target_downregulation’ subpathway or gene set. Subpathway or gene set contained in drug regulation data should exist in input data of parameter ‘subpathway.list’.

drug.spw.p.val.th
Parameter used only when ‘drug.spw.data=“DrugSpwData”‘. According to the threshold of the significant P value set by parameter ‘drug.spw.p.val.th’ (default: 0.05), the drug up-regulation and down-regulatory subpathways were screened.

drug.spw.min.sz
A numeric. The drug regulated subpathways intersects with the subpathways in the subpathway activity profile. Then drugs with less than ‘drug.spw.min.sz’ (default: 10) up- or down-regulated subpathways are removed.

drug.spw.max.sz
A numeric. Similar to parameter ‘drug.spw.min.sz’, drugs with more than ‘drug.spw.max.sz’ (default: Inf) up- or down-regulated subpathways are removed.

weighted.drug.score
A boolean values determines the method for calculating the normalized drug-disease reverse association score of the drug for each sample. ‘weighted.drug.score=TRUE‘ (default): KS random walk statistic with individualized subpathway activity aberrance score as weight was used to calculate the normalized drug-disease reverse association score. ‘weighted.drug.score=FALSE’: Similar to ‘CMap’ (Lamb et al., 2006), no weight is needed, and the normalized drug-disease reverse association score is calculated by the rank of the individualized subpathway activity aberrance score.

nperm
Number of random permutations (default: 1000).

parallel.sz
Number of processors to use when doing the calculations in parallel (default value: 1). If parallel.sz=0, then it will use all available core processors unless we set this argument with a smaller number.

E_FDR
Significance threshold for E_FDR for drugs (default: 0.05)

S_FDR
Significance threshold for S_FDR for drugs (default: 0.001)
Details

PrioSubtypeDrug

First, the function PrioSubtypeDrug uses the ‘GSVA’ or ‘ssgsea’ method to convert the disease gene expression profile into subpathway activity profile. Parameters ‘subpathway.list’, ‘spw.min.sz’ and ‘spw.max.sz’ are used to process the subpathway list data. ‘spw.score.method’ and ‘kcdf’ are used to control the method of constructing the subpathway activity score profile. Individualized subpathway activity aberrance score was estimated using the mean and standard deviation of the Control samples. Subpathways of each cancer sample are ordered in a ranked list according to individualized subpathway activity aberrance score. Next, we calculate the normalized drug-disease reverse association score by enriching drug regulated subpathway tags to the subpathway ranked list. Finally, all drug-regulated subpathways are enriched into each cancer sample to obtain a normalized drug-disease reverse association score matrix. The ‘drug.spw.p.val.th’, ‘drug.spw.min.sz’ and ‘drug.spw.max.sz’ is used to screen the drug regulated subpathway set. If user-defined drug targeting data is used, drug regulated ‘Target_upregulation’ and ‘Target_downregulation’ should already be defined in the data. The ‘weighted.drug.score’ to control the method of calculating the normalized drug-disease reverse association score. Finally, empirical sample-based permutation test procedure to obtain significative cancer subtype specific drugs. For samples containing only cancer and Control, the subpathways are ranked according to the difference in activity between cancer and Control samples. Subsequently, the subpathway set of drug up- and down-regulated is enriched to the ranking list of subpathway to evaluate the normalized drug-disease reverse association score and subpathway-based permutation test procedure to calculate significance. The subpathway list data and drug subpathway associated data set is stored in package ‘SubtypeDrugData’ and can be obtained on [https://github.com/hanjunwei-lab/SubtypeDrugData](https://github.com/hanjunwei-lab/SubtypeDrugData).

Value

A list contains the result table of drug scoring and significance, a subpathway activity score matrix, a normalized drug-disease reverse association score matrix, sample information, and user set parameter information.

Author(s)

Xudong Han, Junwei Han, Chonghui Liu

Examples

```r
require(GSVA)
require(parallel)
## Get simulated breast cancer gene expression profile data.
Geneexp<-get("Geneexp")
## Obtain sample subtype data and calculate breast cancer subtype-specific drugs.
Subtype<-system.file("extdata", "Subtype_labels.cls", package = "SubtypeDrug")

## Subpathway list data and drug subpathway association data
## were stored in packet 'SubtypeDrugData'.
## 'SubtypeDrugData' has been uploaded to the github repository.
## If subpathway list data and drug subpathway association data are needed,
## users can download and install through 'install_github' function and
## set parameter url="hanjunwei-lab/SubtypeDrugData".
```
## After installing and loading package `SubtypeDrugData`,
## users can use the following command to get the data.
## Get subpathway list data.
## If the gene expression profile contains gene Symbol.
## data(SpwSymbolList)
## If the gene expression profile contains gene Entrezid.
## data(SpwEntrezidList)
## Get drug subpathway association data.
## data(DrugSpwData)

## Identify breast subtype-specific drugs.
Subtype_drugs<-PrioSubtypeDrug(Geneexp,Subtype,"Control",SpwSymbolList,drug.spw.data=DrugSpwData,
E_FDR=1,S_FDR=1)

## Identify breast cancer-related drugs in only two types of samples: breast cancer and control.
Cancer<-system.file("extdata", "Cancer_normal_labels.cls", package = "SubtypeDrug")
Disease_drugs<-PrioSubtypeDrug(Geneexp,Cancer,"Control",SpwSymbolList,drug.spw.data=DrugSpwData,
E_FDR=1,S_FDR=1)

## The function PrioSubtypeDrug() can also support user-defined data.
Geneexp<-get("GeneexpT")
UserDS<-get("UserDST")
str(UserDS)

## Need to load gene set data consistent with drug regulation data.
UserGS<-get("UserGST")
str(UserGS)

Drugs<-PrioSubtypeDrug(Geneexp,Cancer,"Control",UserGS,spw.min.sz=1,
  drug.spw.data=UserDS,drug.spw.min.sz=1,
nperm=10,E_FDR=1,S_FDR=1)

---

**Description**

These are function read sample label file (.cls format).

**Usage**

ReadClsFile(file)

**Arguments**

- file: Input sample subtype class vector file in CLS format.

**Details**

ReadClsFile
SpwNetworkData

Value

a list

Author(s)

Xudong Han, Junwei Han, Chonghui Liu

Examples

```r
Subtype <- system.file("extdata", "Subtype_labels.cls", package = "SubtypeDrug")
x <- ReadClsFile(Subtype)
```

---

<table>
<thead>
<tr>
<th>SpwNetworkData</th>
<th>Subpathway network structure data</th>
</tr>
</thead>
</table>

Description

A list to store the network data of the genes contained in the subpathway.

Usage

SpwNetworkData

Format

A list containing 1598 subpathway network.

Examples

```r
data(SpwNetworkData)
```

---

<table>
<thead>
<tr>
<th>Subtype_drugs</th>
<th>Simulation result data</th>
</tr>
</thead>
</table>

Description

The result data of the simulation is generated by the functional OCSSD.

Usage

Subtype_drugs
**Format**

A list containing 8 variables. The variables are as follows:

- Basal Results table for basal subtype
- Her2 Results table for Her2 subtype
- LumA Results table for LumA subtype
- LumB Results table for LumB subtype
- DrugMatrix Drug disease reverse association matrix
- SubpathwayMatrix Subpathway activity matrix
- SampleInformation Cancer sample phenotypic information
- Parameter Parameter of the function OCSSD

**Examples**

```r
# data(Subtype_drugs)
```

---

**UserDS**

*Simulated user-defined drug regulator subpathway dataset*

---

**Description**

The drug regulator subpathway data set is modeled as a case.

**Usage**

`UserDS`

**Format**

A list containing 5 drugs.

**Examples**

```r
data(UserDS)
```
<table>
<thead>
<tr>
<th>UserDST</th>
<th>User-defined drug regulator subpathway dataset for testing</th>
</tr>
</thead>
</table>

**Description**

The drug regulator subpathway data set is modeled as a case.

**Usage**

UserDST

**Format**

A list.

**Examples**

```r
data(UserDST)
```

<table>
<thead>
<tr>
<th>UserGS</th>
<th>Simulated user-defined gene set data</th>
</tr>
</thead>
</table>

**Description**

Gene set data is simulated for case studies.

**Usage**

UserGS

**Format**

A list containing 50 gene sets.

**Examples**

```r
data(UserDS)
```
UserGST

User-defined gene set data for testing

Description
Gene set data is simulated for case studies.

Usage
UserGST

Format
A list.

Examples
data(UserGST)
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