Package ‘immcp’

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Suggests knitr, rmarkdown

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BugReports https://github.com/YuanlongHu/immcp/issues

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Candidate Prescriptions Discovery Based on Pathway Fingerprint

Description

The pathway fingerprint is a method to indicate the profile of significant pathways being influenced by drugs, which may hint drug functions. Through the similarity of pathway fingerprints, the potential relationship between disease and prescription can be found. Ye (2012) <doi: 10.1007/s13238-012-2011-z>.
as.data.frame

Coerce a ScoreResult object into a data frame

Description

Coerce a ScoreResult object into a data frame

Usage

## S4 method for signature 'ScoreResult'
as.data.frame(x, row.names = NULL, optional = FALSE, ...)

Arguments

x
A ScoreResult object
row.names
NULL or a character vector giving the row names for the data frame. Missing values are not allowed.
optional
logical. If TRUE, setting row names and converting column names (to syntactic names: see make.names) is optional. Note that all of R's base package as.data.frame() methods use optional only for column names treatment, basically with the meaning of data.frame(*, check.names = !optional). See also the make.names argument of the matrix method.
...
other arguments

Author(s)

Yuanlong Hu

BasicData-class

Class "BasicData" This class represents the basic input data.

Description

Class "BasicData" This class represents the basic input data.

Slots

BasicData Alist containing basic data.
Key Column name of basic data.
Relationship Relationship.
CompoundAnno Compound ID

Author(s)

Yuanlong Hu
CreateBasicData

Description

Prepare input data.

Usage

CreateBasicData(...)

Arguments

... A data frame from PrepareData.

Value

a list

Author(s)

Yuanlong Hu

Examples

data("drugSample")
drug_herb <- PrepareData(drugSample$drug_herb, col1 = "drug", col2 = "herb")
herb_target <- PrepareData(drugSample$herb_target,
    col1 = "herb", col2 = "target",
    format = "basket", sep = ",")
drug_target <- CreateBasicData(drug_herb, herb_target)

drugResult A demo dataset contains all result.

Description

A demo dataset contains all result.

drugSample A demo dataset contains a sample of herbal prescription.

Description

A demo dataset contains a sample of herbal prescription.
Description

Calculate the pathway fingerprints

Usage

extrFP(drug_target, disease_biomarker, method = "enrich")

# S4 method for signature 'BasicData'
extrFP(drug_target, disease_biomarker, method = "enrich")
extrFP.BasicsData(drug_target, disease_biomarker, method = "enrich")

Arguments

drug_target A data frame or list of drug target.
disease_biomarker A character of disease biomarkers or an order ranked geneList.
method one of "enrich" and "gsea"

Value

ScoreFP object
ScoreFP object

Author(s)

Yuanlong Hu

Examples

data("drugSample")
drug_herb <- PrepareData(drugSample$drug_herb, col1 = "drug", col2 = "herb")
herb_target <- PrepareData(drugSample$herb_target,
    col1 = "herb", col2 = "target",
    format = "basket", sep = ",", )
drug_target <- CreateBasicData(drug_herb, herb_target)
FP <- extrFP(drug_target = drug_target,
    disease_biomarker = drugSample$disease_biomarker,
    method = "enrich")
getDEG

Description
Calculate differentially expressed genes using limma method.

Usage
getDEG(data, pdata, contrasts)

Arguments
- data: A matrix of expression values where rows correspond to genes and columns correspond to samples.
- pdata: A character vector of phenotype.
- contrasts: character vector specifying contrasts

Value
A list

Author(s)
Yuanlong Hu

gxF

Description
Select features related to phenotype using Boruta

Usage
gxF(expr, pdata, level = "gene", withTentative = TRUE, geneset)

Arguments
- expr: A matrix of expression values where rows correspond to genes and columns correspond to samples.
- pdata: A character of phenotype.
- level: one of the gene or pathway
- withTentative: If set to TRUE, Tentative attributes will be also returned.
- geneset: A data frame of geneset containing two columns.
**get_result**

**Value**

A character of features.

**Author(s)**

Yuanlong Hu

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**get_result**

**Description**

Extract a table of the score result

**Usage**

```r
get_result(result, pvalueCutoff = 0.05)
```

**Arguments**

- `result`: an object of class `ScoreResult`.
- `pvalueCutoff`: p-value cutoff.

**Value**

a data.frame

**Author(s)**

Yuanlong Hu

**Examples**

```r
data("drugResult")
res <- drugResult$demoScoreFP
res <- get_result(res)
```
head

Return the First Parts of a ScoreResult Object

Description

Return the First Parts of a ScoreResult Object

Usage

## S4 method for signature 'ScoreResult'
head(x, ...)

Arguments

x A ScoreResult object
...
other arguments

Author(s)

Yuanlong Hu

imm_centr

Computing the centrality of complex networks

Usage

imm_centr(x, ...)

## S4 method for signature 'data.frame'
imm_centr(x)

## S4 method for signature 'ScoreResultNet'
imm_centr(x, drug, node = "target", net = "disease")

imm_centr.data.frame(x, node, net)

imm_centr.ScoreResultNet(x, drug, node, net)
**overlap_pathway**

**Arguments**

- `x`: ScoreResultNet or data.frame object.
- `...`: additional parameters
- `drug`: drug name
- `node`: Nodes that need to be evaluated. one of "disease" and "target.
- `net`: Network. one of "disease" and "target.

**Value**

data.frame or ScoreResultNet object

**Author(s)**

Yuanlong Hu

---

**Description**

Performs set intersection on pathways fingerprints

**Usage**

```r
overlap_pathway(FP, Drug)
```

**Arguments**

- `FP`: A ScoreFP Object
- `Drug`: The drug names

**Value**

a vector or data frame

**Author(s)**

Yuanlong Hu
plot_density

Description

Plot smoothed density estimates for adjusted score

Usage

plot_density(result, drug, fill = "#6495ED")

Arguments

result an object of class ScoreResult.
drug a character of drug name.
fill fill color.

Value

a ggplot

Author(s)

Yuanlong Hu

Examples

## Not run:
data("drugSample")
FP <- extrFP(disease_biomarker = drugSample$disease_biomarker,
  drug_target = drugSample$herb_target,
  geneset = "ImmGenTop150")
res <- score_fp(FP, n=100)
plot_density(res, drug="BAN_XIA_XIE_XIN_TANG")

## End(Not run)
Description

Drug target or pathway network visualization

Usage

```r
plot_network(
  x,
  Drug,
  node_color = c("lightblue", "orange", "red", "green"),
  layout = "layout_nicely",
  manipulation = FALSE,
  ...
)
```

## S4 method for signature 'ScoreResultNet'
```r
plot_network(
  x,
  Drug,
  node_color = c("lightblue", "orange", "red", "green"),
  layout = "layout_nicely",
  manipulation = FALSE,
  node_type = "target",
  background = "drug",
  neighbor = FALSE
)
```

## S4 method for signature 'ScoreFP'
```r
plot_network(
  x,
  Drug,
  node_type = "herb-compound-target",
  node_color = c("lightblue", "orange", "red", "green"),
  layout = "layout_nicely",
  manipulation = FALSE,
  highlight = NULL,
  width = FALSE
)
```

## S4 method for signature 'ScoreResultFP'
```r
plot_network(
  x,
  Drug,
  node_type = "herb-compound-target",
```
node_color = c("lightblue", "orange", "red", "green"),
layout = "layout_nicely",
manipulation = FALSE,
highlight = NULL,
width = FALSE
)

plot_network.ScoreResultNet(
  x,
  Drug,
  node_color = c("lightblue", "orange", "red", "green"),
  layout = "layout_nicely",
  manipulation = FALSE,
  node_type = "target",
  background = "drug",
  neighbor = FALSE
)

plot_network.ScoreFP(
  x,
  Drug,
  node_type = "herb-compound-pathway",
  node_color = c("lightblue", "orange", "red", "green"),
  layout = "layout_nicely",
  manipulation = FALSE,
  highlight = NULL,
  width = FALSE
)

Arguments

- **x**: ScoreFP or ScoreResultNet object
- **Drug**: The name of drug.
- **node_color**: The node color.
- **layout**: Character Name of network layout function to use. Default to "layout_nicely".
- **manipulation**: Whether to edit the network.
- **node_type**: network type. one of "herb-target","herb-compound-target" and "target".
- **background**: one of "drug" or "disease"
- **neighbor**: logical.
- **highlight**: A character vector of gene.
- **width**: A logical. The number of overlapping genes between the two pathways is used as the width of the edges.

Value

visNetwork object
PrepareData

Description

Prepare input format.

Usage

PrepareData(data, col1, col2, format = "single", sep)

Arguments

data A data frame containing interaction information.
col1 A character containing "drug", "herb", "compound", or "target".
col2 A character containing "drug", "herb", "compound", or "target".
format one of "single" or "basket".
sep Separator.

Value

a list

Author(s)

Yuanlong Hu

Examples

data("drugSample")
drug_herb <- PrepareData(drugSample$drug_herb, col1 = "drug", col2 = "herb")
herb_target <- PrepareData(drugSample$herb_target,
col1 = "herb", col2 = "target",
format = "basket", sep = ", ")
Description
parse gmt file to a data.frame

Usage
read_gmt(gmtfile, out_type = "data.frame")

Arguments

gmtfile A GMT file name or URL containing gene sets.
out_type A character vector of object name. one of "data.frame", "list", "GeneSetCollection"

Value
data.frame, list or GeneSetCollection

Author(s)
Yuanlong Hu

Description
Rank the results by rank aggregation methods

Usage
res_rank(..., method = "RRA")

Arguments
...
method rank aggregation method, by default 'RRA', other options are 'min', 'geom.mean', 'mean', 'median' and 'stuart'

Value
a dataframe with two column
ScoreFP-class

Author(s)
Yuanlong Hu

References

ScoreFP-class

Class "ScoreFP" This class represents the pathway fingerprint.

Description
Class "ScoreFP" This class represents the pathway fingerprint.

Slots
Fingerprint pathway fingerprint
FPType pathway fingerprint type
Geneset Geneset name

Author(s)
Yuanlong Hu

ScoreResult-class

Class "ScoreResult"

Description
This class represents the result of score.

Slots
ScoreResult all score reslut.
adj distribution data

Author(s)
Yuanlong Hu
Description

Calculate the pathway fingerprint similarity between disease and prescription.

Usage

score_fp(FP, n = 100, two_tailed = TRUE)

Arguments

- FP: a ScoreFP object
- n: The number of permutations.
- two_tailed: whether returning a two-tailed p-value

Value

ScoreResult

Author(s)

Yuanlong Hu

References

Ye, H., Tang, K., Yang, L., Cao, Z., & Li, Y. (2012). Study of drug function based on similarity of pathway fingerprint. Protein & cell, 3(2), 132-139.

Examples

data("drugResult")
res <- score_fp(drugResult$demoFP, n=100)
res <- get_result(res)
**Description**

Calculate the network score

**Usage**

```r
score_network(Tar, DNet, n = 100, two_tailed = TRUE)
```

**Arguments**

- `Tar`: A BasicData object containing drug target.
- `DNet`: A data frame of disease network containing two columns.
- `n`: The number of times random permutation sampling.
- `two_tailed`: a logical: select a two-tailed p-value.

**Value**

ScoreResultNet object

**Author(s)**

Yuanlong Hu

**Examples**

```r
data("drugSample")
drug_herb <- PrepareData(drugSample$drug_herb, col1 = "drug", col2 = "herb")
herb_target <- PrepareData(drugSample$herb_target,
                           col1 = "herb", col2 = "target",
                           format = "basket", sep = ",", )
drug_target <- CreateBasicData(drug_herb, herb_target)
res <- score_network(Tar = drug_target, DNet = drugSample$disease_network)
res <- get_result(res)
```
**Description**

Calculate the similarity between Drug pathway Fingerprints

**Usage**

`simFP(FP)`

**Arguments**

- **FP** A ScoreFP object

**Value**

a matrix

**Author(s)**

Yuanlong Hu

**Examples**

```r
data("drugResult")
sim_mat <- simFP(drugResult$demoFP)
```

---

**tail**

*Return the last Parts of a ScoreResult Object*

**Description**

Return the last Parts of a ScoreResult Object

**Usage**

```r
## S4 method for signature 'ScoreResult'
tail(x, ...)
```

**Arguments**

- **x** A ScoreResult object
- **...** other arguments
to_df

Author(s)
Yuanlong Hu

Description
Convert list to data.frame

Usage
to_df(list)

Arguments
list a list containing gene sets

Value
data frame

Author(s)
Yuanlong Hu

to_list
to_list

Description
Create a new list from a data.frame of drug target and disease biomarker as input

Usage
to_list(dataframe, input = "single", sep = ", ")

Arguments
dataframe a data frame of 2 column with term/drug and gene
input one of the single or basket
sep When 'input' is 'basket'.

Value
list
**viewpathway**

**Description**

View pathway information.

**Usage**

```r
viewpathway(x, drug, view = "intersect")
```

**Arguments**

- `x`: a ScoreFP object.
- `drug`: character vector of drug name.
- `view`: one of intersect, drug or disease.

**Value**

ScoreResult object

**Author(s)**

Yuanlong Hu

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**write_gmt**

**Description**

prints data frame to a gmt file

**Usage**

```r
write_gmt(geneset, gmt_file)
```

**Arguments**

- `geneset`: A data.frame of 2 column with term/drug and gene
- `gmt_file`: A character of gmt file name.
write_gmt

Value

gmt file

Author(s)

Yuanlong Hu
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