Package 'immcp'

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Title Candidate Prescriptions Discovery Based on Pathway Fingerprint

Version 0.9.1

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>.

License GPL-3

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Suggests knitr, rmarkdown

VignetteBuilder knitr

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

URL https://github.com/YuanlongHu/immcp

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R topics documented:

`immcp-package` *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

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drugResult *A demo dataset contains all result.*

Description

A demo dataset contains all result.

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drugSample *A demo dataset contains a sample of herbal prescription.*

Description

A demo dataset contains a sample of herbal prescription.

---

extrFP *extrFP*

Description

Calculate the pathway fingerprints

Usage

```
extrFP(disease_biomarker, drug_target, method = "enrich", geneset = "KEGG")
```

Arguments

disease_biomarker	A character of disease biomarkers or an order ranked geneList.
drug_target	A data frame or list of drug target.
method	one of "enrich" and "gsea"
geneset	one of "ImmGenTop150" and "KEGG"

Value

ScoreFP object

Author(s)

Yuanlong Hu

Examples

```
data("drugSample")
FP <- extrFP(disease_biomarker = drugSample$disease_biomarker,
             drug_target = drugSample$herb_target,
             method = "enrich",
             geneset = "KEGG")
```

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get_result *get_result*

Description

Extract a table of the score result

Usage

```
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

```
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

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overlap_pathway *overlap_pathway*

Description

Performs set intersection on pathyways fingerprints

Usage

```
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` *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)
```

plot_network *plot_network*

Description

Drug target or pathway network visualization

Usage

```
plot_network(
  x,
  Drug,
  node_color = c("orange", "lightblue"),
  layout = "layout_nicely",
  ...
)

## S4 method for signature 'ScoreResultNet'
plot_network(
  x,
  Drug,
  node_color = c("orange", "lightblue"),
  layout = "layout_nicely",
  node_type = "target"
)

## S4 method for signature 'ScoreFP'
plot_network(
  x,
  Drug,
  node_color = c("orange", "lightblue"),
  layout = "layout_nicely",
  highlight = NULL,
  width = FALSE
)

plot_network.ScoreResultNet(
  x,
  Drug,
  node_color = c("orange", "lightblue"),
  layout = "layout_nicely",
  node_type = "target"
)

plot_network.ScoreFP(
  x,
  Drug,
```

```
  node_color = c("orange", "lightblue"),
  layout = "layout_nicely",
  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".
...	additional parameters
node_type	one of "target" or "all"
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

Author(s)

Yuanlong Hu

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read_gmt *write_gmt*

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

`res_rank` *res_rank*

Description

Rank the results by rank aggregation methods

Usage

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

Arguments

`...`	ScoreResult Object
`method`	rank aggregation method, by defaylt `'RRA'`, other options are `'min'`, `'geom.mean'`, `'mean'`, `'median'` and `'stuart'`

Value

a dataframe with two column

Author(s)

Yuanlong Hu

References

Kolde, R., Laur, S., Adler, P., & Vilo, J. (2012). Robust rank aggregation for gene list integration and meta-analysis. Bioinformatics, 28(4), 573-580.

`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

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score_fp *score_fp*

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)
```

`score_network` *score_network*

Description

Calculate the network score

Usage

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

Arguments

`Tar`	A list 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

```
data("drugSample")
res <- score_network(Tar = drugSample$herb_target, DNet = drugSample$disease_network)
res <- get_result(res)
```

simFP *simFP*

Description

Calculate the similarity between Drug pathway Fingerprints

Usage

```
simFP(FP)
```

Arguments

FP	A ScoreFP object

Value

a matrix

Author(s)

Yuanlong Hu

Examples

```
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

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

Arguments

x	A ScoreResult object
...	other arguments

Author(s)

Yuanlong Hu

`write_gmt` *write_gmt*

Description

prints data frame to a gmt file

Usage

```
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.

Value

gmt file

Author(s)

Yuanlong Hu

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