Package 'lilikoi2'

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Type Package

Title Metabolomics Personalized Pathway Analysis Tool

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Description More about what it does (maybe more than one line)
Use four spaces when indenting paragraphs within the Description.

Imports caret,
corrplot,
devtools,
dplyr,
e1071,
gbm,
ggplot2,
glmnet,
hash,
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Matrix,
pamr,
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pROC,
randomForest,
reshape2,
RWeka,
stringr

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Encoding UTF-8

LazyData true

RoxygenNote 7.0.2

R topics documented:

`featuresSelection` *A featuresSelection Function*

Description

This function allows you to reduce the pathway diemsion using xxxx

Usage

```
featuresSelection(PDSmatrix, threshold = 0.5, method = "info")
```

Arguments

`PDSmatrix`	from PDSfun function

Examples

```
selected_Pathways_Weka= featuresSelection(PDSmatrix)
featuresSelection(PDSmatrix)
```

`lilikoi_pathway`

Arguments

`gene.data`	gene expression dataset
`cpd.data`	metabolite compounds dataset
`pathway.id`	pathway id

Value

Pathview visualization output

Examples

```
lilikoi_pathview(gene.data, cpd.data, pathway.id)
```

lilikoi_preproc *A preprocessing function.*

Description

This function is used to preprocess data via normalization and imputation. It provides three normalization methods: standard normalization, quantile normalization and median fold normalization. It also enables KNN imputation.

Usage

```
lilikoi_preproc(
  inputdata = Metadata,
  method = c("standard", "quantile", "median", "knn")
)
```

Arguments

inputdata	An expression data frame with samples in the rows, metabolites in the columns
method	The method to be used to process data, including

Value

a processed dataset with samples in the rows, metabolites in the columns.

Examples

```
preproc(inputdata=Metadata, method="standard")
```

lilikoi_prognosis *Pathway-based prognosis model*

Description

Pathway-based prognosis model

Usage

```
lilikoi_prognosis(
  PDSmatrix,
  event,
  time,
  exprdata,
  percent,
  alpha,
  nfold,
  method
)
```

Arguments

PDSmatrix	Pathway deregulation score matrix‘1àQDF‘
event	survival event
time	survival time
exprdata	dataset for penalization
percent	train-test separation percentage
alpha	denote which penalization method to use.
nfold	fold number for cross validation
method	determine the prognosis index

Examples

```
lilikoi_prognosis(PDSmatrix, event, time, exprdata, percent, alpha, nfold, method)
```

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lilikoi_regression *Metabolite-pathway regression*

Description

Perform single variate linear regression between selected pathways and each of their metabolites.

Usage

```
lilikoi_regression(
  input = "Aminoacyl-tRNA Biosynthesis",
  PDSmatrix,
  selected_Pathways_Weka,
  Metabolite_pathway_table
)
```

Arguments

input	Pathway name
PDSmatrix	Pathway deregulation score matrix
selected_Pathways_Weka	Selected top pathways from the featureSelection function
Metabolite_pathway_table	Metabolites mapping table

Value

A list of regression summaries.

Examples

```
lilikoi_regression(input="Aminoacyl-tRNA Biosynthesis", PDSmatrix, selected_Pathways_Weka, Metabolite_pathwa
```

Loaddata *A Loaddata Function*

Description

This function allows you to load your metabolomics data.

Usage

```
Loaddata(filename)
```

Arguments

Your	file name.

Examples

```
Loaddata("data_format.csv")
Loaddata()
```

machine_learning *A machine learning Function*

Description

This function for classification using 8 different machine learning algorithms and it plot the ROC curves and the AUC, SEN, and specificty

Usage

```
machine_learning(PDSmatrix, selected_Pathways_Weka)
```

Arguments

PDSmatrix	from PDSfun function and selected_Pathways_Weka from featuresSelection function

Examples

```
machine_learning(PDSmatrix,selected_Pathways_Weka)
machine_learning(PDSmatrix,selected_Pathways_Weka)
```

`MetaTOpathway` *A MetaTOpathway Function*

Description

This function allows you to convert your metabolites id such as names, kegg ids, pubchem ids. into pathways. Metabolites which have not pathways will be excluded from any downstream analysis make sure that you have three database files which are used for exact and fuzzy matching: cmpd_db.rda, syn_nms_db.rda and Sijia_pathway.rda This function was modified version of the name.match function in the below link: https://github.com/cangfengzhe/Metabo/blob/master/MetaboAnalyst/website/nar

Usage

```
MetaTOpathway(q.type, hmdb = T, pubchem = T, chebi = F, kegg = T, metlin = F)
```

Arguments

`q.type`	The type of the metabolites id such as 'name', 'kegg', 'hmdb','pubchem'

Examples

```
Metabolite_pathway_table=MetaTOpathway('name')
MetaTOpathway()
```

`model_adjustment` *Model Adjustemnt function using clinical factors*

Description

This function for adjusted the best performed model using the clinical factors inserted by the user It plots ROC for three models: model1 build using only seelcted pathways, model2 build using clinical factors and model3 build using selected pathways and the clinical factors

Usage

```
model_adjustment(
  result,
  PDSmatrix,
  selected_Pathways_Weka,
  clinical_factors_data,
  factors
)
```

Arguments

PDSmatrix	the PDS matrix geneerated using PDSfun function
selected_Pathways_Weka	selected pathway using WEKA algorithm geneerated from featuresSelection function
clinical_factors_data	the metadata for the samples
factors	which the users want to add to the model

Examples

```
model_adjustment(result,PDSmatrix,selected_Pathways_Weka,clinical_factors_data,factors=c('Age','Race'))
model_adjustment(result,PDSmatrix,selected_Pathways_Weka,clinical_factors_data,factors=c('Age','Race'))
```

PDSfun *A PDSfun Function*

Description

This function allows you to compute Pathway Desregulation Score deriving make sure that you have the below database for the metabolites and pathway list: meta_path.RData

Usage

```
PDSfun(qvec)
```

Arguments

qvec	This is the Metabolite_pathway_table from MetaTOpathway function. This table includes the metabolites ids and the its corssponding hmdb ids

Examples

```
PDSmatrix= PDSfun(Metabolite_pathway_table)
PDSfun(Metabolite_pathway_table)
```

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