Package 'Rtpca'

July 12, 2025

Title Thermal proximity co-aggregation with R

Version 1.19.0

Description R package for performing thermal proximity co-aggregation analysis with thermal proteome profiling datasets to analyse protein complex assembly and (differential) protein-protein interactions across conditions.

License GPL-3

Encoding UTF-8

VignetteBuilder knitr

LazyData false

biocViews Software, Proteomics, DataImport

BugReports https://support.bioconductor.org/

Depends R (>= 4.0.0), stats, dplyr, tidyr

Imports Biobase, methods, ggplot2, pROC, fdrtool, splines, utils, tibble

Suggests knitr, BiocStyle, TPP, testthat, rmarkdown

RoxygenNote 7.1.0

git_url https://git.bioconductor.org/packages/Rtpca

git_branch devel

git_last_commit c9ed1d1

git_last_commit_date 2025-04-15

Repository Bioconductor 3.22

Date/Publication 2025-07-11

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```
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```

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Value

a vector of common features across replicates

Examples

```
m1 <- matrix(1:12, ncol = 4)
m2 <- matrix(2:13, ncol = 4)
m3 <- matrix(c(2:10, 1:7), ncol = 4)

rownames(m1) <- 1:3
rownames(m2) <- 2:4
rownames(m3) <- 2:5

mat_list <- list(
    m1, m2, m3
)

ppi_anno <- tibble(
    x = "2",
    y = "3",
    combined_score = 700,
    pair = "2:3")

tpcaObj <- runTPCA(
    objList = mat_list,
    complexAnno = NULL,
    ppiAnno = ppi_anno
)

CommonFeatures(tpcaObj)
```

ComplexAnnotation,tpcaResult-method

Extract ComplexAnnotation

Description

Extract ComplexAnnotation

Usage

```
## S4 method for signature 'tpcaResult'
ComplexAnnotation(object)
```

Arguments

object	and object of class tpcaResult

Value

a data frame containing the complex annotation

Examples

```
m1 <- matrix(1:12, ncol = 4)
m2 <- matrix(2:13, ncol = 4)
m3 <- matrix(c(2:10, 1:7), ncol = 4)

rownames(m1) <- 1:3
rownames(m2) <- 2:4
rownames(m3) <- 2:5

mat_list <- list(
    m1, m2, m3
)
tpcaObj <- new("tpcaResult", ObjList = mat_list)
ComplexAnnotation(tpcaObj)
```

ComplexBackgroundDistributionList,tpcaResult-method

Extract ComplexBackgroundDistributionList

Description

Extract ComplexBackgroundDistributionList

Usage

```
## S4 method for signature 'tpcaResult'
ComplexBackgroundDistributionList(object)
```

Arguments

object	and object of class tpcaResult

Value

a list of data frames containing distances of random complexes with different number of members

Examples

```
m1 <- matrix(1:12, ncol = 4)
m2 <- matrix(2:13, ncol = 4)
m3 <- matrix(c(2:10, 1:7), ncol = 4)

rownames(m1) <- 1:3
rownames(m2) <- 2:4
rownames(m3) <- 2:5
```

```
mat_list <- list(
    m1, m2, m3
)
tpcaObj <- new("tpcaResult", ObjList = mat_list)
ComplexBackgroundDistributionList(tpcaObj)
```

ComplexRocTable,tpcaResult-method
Extract ComplexRocTable

Description

Extract ComplexRocTable

Usage

```
## S4 method for signature 'tpcaResult'
ComplexRocTable(object)
```

Arguments

object	and object of class tpcaResult

Value

a data frame containing a complex analysis roc table

Examples

```
m1 <- matrix(1:12, ncol = 4)
m2 <- matrix(2:13, ncol = 4)
m3 <- matrix(c(2:10, 1:7), ncol = 4)

rownames(m1) <- 1:3
rownames(m2) <- 2:4
rownames(m3) <- 2:5

mat_list <- list(
    m1, m2, m3
)
tpcaObj <- new("tpcaResult", ObjList = mat_list)
ComplexRocTable(tpcaObj)
```

ContrastCondName,tpcaResult-method
Extract ContrastCondName

Description

Extract ContrastCondName

Usage

```
## S4 method for signature 'tpcaResult'
ContrastCondName(object)
```

Arguments

object	and object of class tpcaResult

Value

a character string describing the contrast condition

Examples

```
tpcaObj <- new("tpcaResult")
ContrastCondName(tpcaObj)
```

ContrastDistMat,tpcaResult-method
Extract ContrastDistMat

Description

Extract ContrastDistMat

Usage

```
## S4 method for signature 'tpcaResult'
ContrastDistMat(object)
```

Arguments

object	an object of class tpcaResult

Value

a matrix containing the constrast distance matrix of all pariwise protein-protein melting curve distances computed from a TPP experiment

Examples

```
m1 <- matrix(1:12, ncol = 4)
m2 <- matrix(2:13, ncol = 4)
m3 <- matrix(c(2:10, 1:7), ncol = 4)

rownames(m1) <- 1:3
rownames(m2) <- 2:4
rownames(m3) <- 2:5

mat_list <- list(
    m1, m2, m3
)
tpcaObj <- new("tpcaResult", ObjList = mat_list)
ContrastDistMat(tpcaObj)
```

ContrastList,tpcaResult-method

Extract ContrastList

Description

Extract ContrastList

Usage

```
## S4 method for signature 'tpcaResult'
ContrastList(object)
```

Arguments

`object`	an object of class tpcaResult

Value

an object list containing TPP data

Examples

```
m1 <- matrix(1:12, ncol = 4)
m2 <- matrix(2:13, ncol = 4)
m3 <- matrix(c(2:10, 1:7), ncol = 4)

rownames(m1) <- 1:3
rownames(m2) <- 2:4
rownames(m3) <- 2:5

mat_list <- list(
    m1, m2, m3
)
tpcaObj <- new("tpcaResult", ObjList = mat_list)
ContrastList(tpcaObj)
```

createDistMat *Create distance matrix of all vs all protein melting profiles*

Description

Create distance matrix of all vs all protein melting profiles

Usage

```
createDistMat(
  objList,
  rownameCol = NULL,
  summaryMethodStr = "median",
  distMethodStr = "euclidean"
)
```

Arguments

objList	list of objects suitable for the analysis, currently allowed classes of objects are: matrices, data.frames, tibbles and ExpressionSets
rownameCol	in case the input objects are tibbles this parameter takes in the name (character) of the column specifying protein names or ids
summaryMethodStr	character string indicating a method to use to summarize measurements across replicates, default is "median", other options are c("mean", "rbind")
distMethodStr	method to use within dist function, default is 'euclidean'

Value

a distance matrix of all pairwise protein melting profiles

Examples

```
library(Biobase)

m1 <- matrix(1:12, ncol = 4)
m2 <- matrix(2:13, ncol = 4)
m3 <- matrix(c(2:10, 1:7), ncol = 4)

rownames(m1) <- 1:3
rownames(m2) <- 2:4
rownames(m3) <- 2:5

colnames(m1) <- paste0("X", 1:4)
colnames(m2) <- paste0("X", 1:4)
colnames(m3) <- paste0("X", 1:4)

mat_list <- list(
    m1, m2, m3
)

createDistMat(mat_list)
```

```
expr1 <- ExpressionSet(m1)
expr2 <- ExpressionSet(m2)
expr3 <- ExpressionSet(m3)

exprSet_list <- list(
    expr1, expr2, expr3
)

createDistMat(exprSet_list)
```

`CtrlCondName,tpcaResult-method`
Extract CtrlCondName

Description

Extract CtrlCondName

Usage

```
## S4 method for signature 'tpcaResult'
CtrlCondName(object)
```

Arguments

`object`	and object of class tpcaResult

Value

a character string describing the control condition

Examples

```
tpcaObj <- new("tpcaResult")
CtrlCondName(tpcaObj)
```

`diffTpcaResultTable,tpcaResult-method`
Extract diffTpcaResultTable

Description

Extract diffTpcaResultTable

Usage

```
## S4 method for signature 'tpcaResult'
diffTpcaResultTable(object)
```

Arguments

object	an object of class tpcaResult

Value

a data frame containing the results from a diffTpca analysis

Examples

```
m1 <- matrix(1:12, ncol = 4)
m2 <- matrix(2:13, ncol = 4)
m3 <- matrix(c(2:10, 1:7), ncol = 4)

rownames(m1) <- 1:3
rownames(m2) <- 2:4
rownames(m3) <- 2:5

mat_list <- list(
    m1, m2, m3
)
tpcaObj <- new("tpcaResult", ObjList = mat_list)
diffTpcaResultTable(tpcaObj)
```

DistMat,tpcaResult-method

Extract DistMat

Description

Extract DistMat

Usage

```
## S4 method for signature 'tpcaResult'
DistMat(object)
```

Arguments

object	an object of class tpcaResult

Value

a matrix containing the distance matrix of all pariwise protein-protein melting curve distances computed from a TPP experiment

Examples

```
m1 <- matrix(1:12, ncol = 4)
m2 <- matrix(2:13, ncol = 4)
m3 <- matrix(c(2:10, 1:7), ncol = 4)

rownames(m1) <- 1:3
rownames(m2) <- 2:4
```

```
rownames(m3) <- 2:5

mat_list <- list(
    m1, m2, m3
)
tpcaObj <- new("tpcaResult", ObjList = mat_list)
DistMat(tpcaObj)
```

DistMethod,tpcaResult-method

Extract DistMethod

Description

Extract DistMethod

Usage

```
## S4 method for signature 'tpcaResult'
DistMethod(object)
```

Arguments

object	and object of class tpcaResult

Value

a character string of the dist method

Examples

```
tpcaObj <- new("tpcaResult")
DistMethod(tpcaObj)
```

ObjList,tpcaResult-method

Extract ObjList

Description

Extract ObjList

Usage

```
## S4 method for signature 'tpcaResult'
ObjList(object)
```

Arguments

object	an object of class tpcaResult

Value

an object list containing TPP data

Examples

```
m1 <- matrix(1:12, ncol = 4)
m2 <- matrix(2:13, ncol = 4)
m3 <- matrix(c(2:10, 1:7), ncol = 4)

rownames(m1) <- 1:3
rownames(m2) <- 2:4
rownames(m3) <- 2:5

mat_list <- list(
    m1, m2, m3
)
tpcaObj <- new("tpcaResult", ObjList = mat_list)
ObjList(tpcaObj)
```

---

ori_et_al_complexes_df

Data frame of annotated protein complexes by Ori et al.

Description

data frame assigning proteins to annotated protein complexes

Usage

```
data("ori_et_al_complexes_df")
```

Format

data frame with columns ensembl_id, protein and id (complex identifier)

References

Ori et al. (2016), Genome Biology, 17, 47

Examples

```
data("ori_et_al_complexes_df")
```

ori_et_al_complex_ppis

Data frame of eukaryotic protein-protein interactions inferred from annotated protein complexes by Ori et al. and StringDB interations with a combined score of at least 900

Description

data frame assigning proteins to (in)directly interacting proteins within protein complexes

Usage

```
data("ori_et_al_complex_ppis")
```

Format

data frame with columns complex_name, x, y, pair (unique pair id)

References

Ori et al. (2016), Genome Biology, 17, 47; Jensen et al. (2009), Nucleic Acids Research, 37, D412–D416

Examples

```
data("ori_et_al_complex_ppis")
```

plotComplexRoc *Plot Complex ROC curve*

Description

Plots a ROC curve representing how well a given TPP dataset recovers annotated proteins complexes. The ROC curve is generated based on the supplied protein complex annotation specificity is assessed by comparing the given complex annotation to random permutations of that table, i.e. proteins randomly grouped together.

Usage

```
plotComplexRoc(tpcaObj, computeAUC = FALSE)
```

Arguments

tpcaObj	tpcaResult object
computeAUC	logical parameter indicating whether area under the ROC should be computed and indicated in the lower right corner of the plot

Value

ggplot object of a receiver operating curve (ROC)

Examples

```
rocTab = data.frame(
    TPR = c(0, 0.1, 0.2, 0.4, 0.5, 0.7, 0.9, 1),
    FPR = c(0, 0.05, 0.1, 0.2, 0.5, 0.7, 0.9, 1)
)

tpcaTest <- new(
    "tpcaResult",
    ComplexRocTable = rocTab)

plotComplexRoc(tpcaTest)
```

`plotDiffTpcaVolcano` *Plot differential TPCA analysis results*

Description

Plot differential TPCA analysis results

Usage

```
plotDiffTpcaVolcano(
  tpcaObj,
  alpha = 0.1,
  setXLim = FALSE,
  xlimit = c(-0.75, 0.75)
)
```

Arguments

`tpcaObj`	a tpcaObj after having performed a differential analysis, see `runDiffTPCA`
`alpha`	significance level / FDR at which null hypothesis should be rejected
`setXLim`	logical determining whether x-axis limits should be set according to xlimit
`xlimit`	numeric vector with two elements determing the x-axis limits, only is implemented if setXLim is set to TRUE

Value

ggplot displaying a volcano plot

Examples

```
library(dplyr)
library(Biobase)

m1 <- matrix(1:28, ncol = 4)
m2 <- matrix(2:25, ncol = 4)
m3 <- matrix(c(2:10, 1:19), ncol = 4)

rownames(m1) <- 1:7
rownames(m2) <- 3:8
```

```
rownames(m3) <- 2:8

mat_list <- list(
    m1, m2, m3
)

c1 <- matrix(29:2, ncol = 4)
c2 <- matrix(26:3, ncol = 4)
c3 <- matrix(c(11:3, 20:2), ncol = 4)

rownames(c1) <- 1:7
rownames(c2) <- 3:8
rownames(c3) <- 2:8

contrast_list <- list(
    c1, c2, c3
)

ppi_anno <- tibble(
    x = c("3", "3"),
    y = c("5", "7"),
    pair = c("3:5", "3:7"))

ref_df <- tibble(
    pair = c("3:5", "3:7"),
    valueC2 = c(4, 8)
)

diff_tpca <- runDiffTPCA(
  mat_list, contrast_list, ppiAnno = ppi_anno)

plotDiffTpcaVolcano(diff_tpca)
```

`plotPPiProfiles` *Plot thermal profile of protein pairs*

Description

Plot thermal profile of protein pairs

Usage

```
plotPPiProfiles(tpcaObj, pair, splinesDf = 4)
```

Arguments

`tpcaObj`	a tpcaObj after having performed a differential analysis, see `runDiffTPCA`
`pair`	character vector of one or more protein names
`splinesDf`	numeric, degree of freedom of the spline fit to the melting curves

Value

ggplot displaying the thermal profile of a protein pair across conditions

Examples

```
library(Biobase)

set.seed(12)
m1 <- matrix(rnorm(50), ncol = 10)
m2 <- matrix(rnorm(50), ncol = 10)

rownames(m1) <- letters[1:5]
rownames(m2) <- letters[1:5]

colnames(m1) <- paste("fc", 1:10, sep = "_")
colnames(m2) <- paste("fc", 1:10, sep = "_")

pheno <- data.frame(
    temperature = seq(37, 67, length.out = 10))
rownames(pheno) <- paste("fc", 1:10, sep = "_")

eset1 <- ExpressionSet(
    assayData = m1,
    phenoData = AnnotatedDataFrame(pheno)
)

eset2 <- ExpressionSet(
    assayData = m2,
    phenoData = AnnotatedDataFrame(pheno)
)

tpcaObj <- new("tpcaResult",
               ObjList = list(eset1),

ContrastList = list(eset2),
                CtrlCondName = "control",
                ContrastCondName = "treatment")

plotPPiProfiles(tpcaObj, pair = c("b", "d"))
```

`plotPPiRoc` *Plot PPI ROC curve*

Description

Plot PPI ROC curve

Usage

```
plotPPiRoc(tpcaObj, computeAUC = FALSE)
```

Arguments

`tpcaObj`	tpcaResult object
`computeAUC`	logical parameter indicating whether area under the ROC should be computed and indicated in the lower right corner of the plot

Value

ggplot object of a receiver operating curve (ROC)

Examples

```
rocTab = data.frame(
    TPR = c(0, 0.1, 0.2, 0.4, 0.5, 0.7, 0.9, 1),
    FPR = c(0, 0.05, 0.1, 0.2, 0.5, 0.7, 0.9, 1)
)

tpcaTest <- new(
    "tpcaResult",
    PPiRocTable = rocTab)

plotPPiRoc(tpcaTest)
```

---

plotTpcaVolcano *Plot TPCA analysis results*

Description

Plot TPCA analysis results

Usage

```
plotTpcaVolcano(tpcaObj, alpha = 0.1)
```

Arguments

tpcaObj	a tpcaObj after having performed a differential analysis, see runDiffTPCA
alpha	significance level / FDR at which null hypothesis should be rejected

Value

ggplot displaying a volcano plot

Examples

```
library(dplyr)
library(Biobase)

m1 <- matrix(1:28, ncol = 4)
m2 <- matrix(2:25, ncol = 4)
m3 <- matrix(c(2:10, 1:19), ncol = 4)

rownames(m1) <- 1:7
rownames(m2) <- 3:8
rownames(m3) <- 2:8

mat_list <- list(
    m1, m2, m3
)
```

```
complex_anno <- tibble(
    protein = c("3", "4", "5",
       "4", "5", "6", "7"),
    id = c(rep("1", 3), rep("2", 4)),
    count = c(rep(3, 3), rep(4, 4)))

tpca_result <- runTPCA(
  mat_list, complexAnno = complex_anno)

plotTpcaVolcano(tpca_result)
```

PPiAnnotation,tpcaResult-method
Extract PPiAnnotation

Description

Extract PPiAnnotation

Usage

```
## S4 method for signature 'tpcaResult'
PPiAnnotation(object)
```

Arguments

object	and object of class tpcaResult

Value

a data frame containing the results from a tpca analysis

Examples

```
m1 <- matrix(1:12, ncol = 4)
m2 <- matrix(2:13, ncol = 4)
m3 <- matrix(c(2:10, 1:7), ncol = 4)

rownames(m1) <- 1:3
rownames(m2) <- 2:4
rownames(m3) <- 2:5

mat_list <- list(
    m1, m2, m3
)
tpcaObj <- new("tpcaResult", ObjList = mat_list)
PPiAnnotation(tpcaObj)
```

PPiRocTable,tpcaResult-method
Extract PPiRocTable

Description

Extract PPiRocTable

Usage

```
## S4 method for signature 'tpcaResult'
PPiRocTable(object)
```

Arguments

object	an object of class tpcaResult

Value

a data frame containing the results from a tpca analysis

Examples

```
m1 <- matrix(1:12, ncol = 4)
m2 <- matrix(2:13, ncol = 4)
m3 <- matrix(c(2:10, 1:7), ncol = 4)

rownames(m1) <- 1:3
rownames(m2) <- 2:4
rownames(m3) <- 2:5

mat_list <- list(
    m1, m2, m3
)
tpcaObj <- new("tpcaResult", ObjList = mat_list)
PPiRocTable(tpcaObj)
```

PPiRocTableAnno,tpcaResult-method
Extract PPiRocTableAnno

Description

Extract PPiRocTableAnno

Usage

```
## S4 method for signature 'tpcaResult'
PPiRocTableAnno(object)
```

Arguments

object	an object of class tpcaResult

Value

a data frame containing annotation information for PPiRocTable

Examples

```
m1 <- matrix(1:12, ncol = 4)
m2 <- matrix(2:13, ncol = 4)
m3 <- matrix(c(2:10, 1:7), ncol = 4)

rownames(m1) <- 1:3
rownames(m2) <- 2:4
rownames(m3) <- 2:5

mat_list <- list(
    m1, m2, m3
)
tpcaObj <- new("tpcaResult", ObjList = mat_list)
PPiRocTableAnno(tpcaObj)
```

---

runDiffTPCA *Run differential TPCA analysis*

Description

Run differential TPCA analysis

Usage

```
runDiffTPCA(
  objList,
  contrastList,
  ctrlCondName = "control",
  contrastCondName = "treatment",
  ppiAnno = NULL,
  complexAnno = NULL,
  rownameCol = NULL,
  summaryMethodStr = "median",
  distMethodStr = "euclidean",
  n = 10000,
  p_adj_method = "BH"
)
```

Arguments

objList	input list of objects, e.g. ExpressionSets retrieved after TPP data import or matrices or data frames
contrastList	input list of objects for comparison at e.g. different treatment condtion, same file formats work as for objList

ctrlCondName	character string indicating the name of the control condition, default is "control"
contrastCondName	character string indicating the name of the contrast condition, default is "treatment"
ppiAnno	data frame annotation known protein-protein interactions (PPI) to test
complexAnno	data frame annotating known protein complexes of interest to test
rownameCol	in case the input objects are tibbles this parameter takes in the name (character) of the column specifying protein names or ids
summaryMethodStr	character string indicating a method to use to summarize measurements across replicates, default is "median", other options are c("mean", "rbind")
distMethodStr	method to use within dist function, default is 'euclidean'
n	number of random protein pair draws to obtain empirical p-value, default is 10000
p_adj_method	method to be used for multiple testing adjusment, default is "BH"

Value

an object of class tpcaResult with the following slots: 1) ObjList: containing the supplied list of objects

Examples

```
library(dplyr)
library(Biobase)

m1 <- matrix(1:28, ncol = 4)
m2 <- matrix(2:25, ncol = 4)
m3 <- matrix(c(2:10, 1:19), ncol = 4)

rownames(m1) <- 1:7
rownames(m2) <- 3:8
rownames(m3) <- 2:8

mat_list <- list(
    m1, m2, m3
)

c1 <- matrix(29:2, ncol = 4)
c2 <- matrix(26:3, ncol = 4)
c3 <- matrix(c(11:3, 20:2), ncol = 4)

rownames(c1) <- 1:7
rownames(c2) <- 3:8
rownames(c3) <- 2:8

contrast_list <- list(
    c1, c2, c3
)

ppi_anno <- tibble(
    x = c("3", "3"),
    y = c("5", "7"),
```

```
    pair = c("3:5", "3:7"))

ref_df <- tibble(
    pair = c("3:5", "3:7"),
    valueC2 = c(4, 8)
)

diff_tpca <- Rtpca:::runDiffTPCA(
  mat_list, contrast_list, ppiAnno = ppi_anno)
```

---

runTPCA *Run the TPCA analysis*

Description

Run the TPCA analysis

Usage

```
runTPCA(
  objList,
  complexAnno = NULL,
  ppiAnno = NULL,
  rownameCol = NULL,
  summaryMethodStr = "median",
  distMethodStr = "euclidean",
  doRocAnalysis = TRUE,
  minCount = 3,
  nSamp = 10000,
  p_adj_method = "BH"
)
```

Arguments

objList	inout list of objects, e.g. ExpressionSets retrieved after TPP data import or matrices or data frames
complexAnno	data frame annotating known protein complexes of interest to test
ppiAnno	data frame annotation known protein-protein interactions (PPI) to test
rownameCol	in case the input objects are tibbles this parameter takes in the name (character) of the column specifying protein names or ids
summaryMethodStr	character string indicating a method to use to summarize measurements across replicates, default is "median", other options are c("mean", "rbind")
distMethodStr	method to use within dist function, default is 'euclidean'
doRocAnalysis	logical indicating whether a ROC analysis should be performed which can be used to assess the predictive power of the dataset for protein-protein interactions / protein complexes based on distanc between melting curves of protein interactions partners

minCount	integer indicating how many subunits of a complex should be qunatified to inlucde it into the analysis, default is 3
nSamp	integer indicating the number of random samples which should be performed to estimate empirical null distributions, default is 10000
p_adj_method	character string indicating a valid method to be used for multiple testing adjusment, default is "BH" which makes p.adjust use benjamini-hochberg, for additional options check ?p.adjust

Value

an object of class tpcaResult with the following slots: 1) ObjList: containing the supplied list of objects

Examples

```
m1 <- matrix(1:12, ncol = 4)
m2 <- matrix(2:13, ncol = 4)
m3 <- matrix(c(2:10, 1:7), ncol = 4)

rownames(m1) <- 1:3
rownames(m2) <- 2:4
rownames(m3) <- 2:5

colnames(m1) <- paste0("X", 1:4)
colnames(m2) <- paste0("X", 1:4)
colnames(m3) <- paste0("X", 1:4)

mat_list <- list(
    m1, m2, m3
)

ppi_anno <- tibble(
    x = "2",
    y = "3",
    combined_score = 700,
    pair = "2:3")

runTPCA(
    objList = mat_list,
    complexAnno = NULL,
    ppiAnno = ppi_anno
)
```

SetCommonFeatures,tpcaResult-method
Set CommonFeatures

Description

Set CommonFeatures

Usage

```
## S4 method for signature 'tpcaResult'
SetCommonFeatures(object, commonFeatures)
```

Arguments

object	and object of class tpcaResult
commonFeatures	a vector of characters indicating the common features across replicates

Value

a vector of common features across replicates

Examples

```
m1 <- matrix(1:12, ncol = 4)
m2 <- matrix(2:13, ncol = 4)
m3 <- matrix(c(2:10, 1:7), ncol = 4)

rownames(m1) <- 1:3
rownames(m2) <- 2:4
rownames(m3) <- 2:5

mat_list <- list(
    m1, m2, m3
)

tpcaObj <- new("tpcaResult", ObjList = mat_list)
SetCommonFeatures(tpcaObj, c("2", "3"))
```

SetComplexAnnotation,tpcaResult-method
Set ComplexAnnotation

Description

Set ComplexAnnotation

Usage

```
## S4 method for signature 'tpcaResult'
SetComplexAnnotation(object, df)
```

Arguments

object	an object of class tpcaResult
df	data frame containing complex annotation

Value

an object of class tpcaResult

Examples

```
m1 <- matrix(1:12, ncol = 4)
m2 <- matrix(2:13, ncol = 4)
m3 <- matrix(c(2:10, 1:7), ncol = 4)

rownames(m1) <- 1:3
rownames(m2) <- 2:4
rownames(m3) <- 2:5

mat_list <- list(
    m1, m2, m3
)
tpcaObj <- new("tpcaResult", ObjList = mat_list)
SetComplexAnnotation(tpcaObj, data.frame(id = "complex1"))
```

SetComplexBackgroundDistributionList,tpcaResult-method
Set ComplexBackgroundDistributionList

Description

Set ComplexBackgroundDistributionList

Usage

```
## S4 method for signature 'tpcaResult'
SetComplexBackgroundDistributionList(object, lt)
```

Arguments

object	an object of class tpcaResult
lt	a list of data frames containing distances of random complexes with different number of members

Value

an object of class tpcaResult

Examples

```
m1 <- matrix(1:12, ncol = 4)
m2 <- matrix(2:13, ncol = 4)
m3 <- matrix(c(2:10, 1:7), ncol = 4)

rownames(m1) <- 1:3
rownames(m2) <- 2:4
rownames(m3) <- 2:5

mat_list <- list(
    m1, m2, m3
)
tpcaObj <- new("tpcaResult", ObjList = mat_list)
SetComplexBackgroundDistributionList(tpcaObj,
  list('3' = data.frame(pair = "A:B")))
```

SetComplexRocTable,tpcaResult-method
Set ComplexRocTable

Description

Set ComplexRocTable

Usage

```
## S4 method for signature 'tpcaResult'
SetComplexRocTable(object, df)
```

Arguments

object	and object of class tpcaResult
df	data.frame containg ComplexRocTable to set

Value

a data frame containing the results from a tpca analysis

Examples

```
m1 <- matrix(1:12, ncol = 4)
m2 <- matrix(2:13, ncol = 4)
m3 <- matrix(c(2:10, 1:7), ncol = 4)

rownames(m1) <- 1:3
rownames(m2) <- 2:4
rownames(m3) <- 2:5

mat_list <- list(
    m1, m2, m3
)
tpcaObj <- new("tpcaResult", ObjList = mat_list)
SetComplexRocTable(tpcaObj, data.frame(FPR = 1, TPR = 1))
```

SetContrastCondName,tpcaResult-method
Set ContrastCondName

Description

Set ContrastCondName

Usage

```
## S4 method for signature 'tpcaResult'
SetContrastCondName(object, name)
```

Arguments

object	an object of class tpcaResult
name	a character string describing the contrast condition

Value

an object of class tpcaResult

Examples

```
tpcaObj <- new("tpcaResult")
SetContrastCondName(tpcaObj, "DMSO")
```

SetContrastDistMat,tpcaResult-method
Set ContrastDistMat

Description

Set ContrastDistMat

Usage

```
## S4 method for signature 'tpcaResult'
SetContrastDistMat(object, mat)
```

Arguments

object	and object of class tpcaResult
mat	matrix containg contrast distance matrix to set

Value

a data frame containing the results from a tpca analysis

Examples

```
m1 <- matrix(1:12, ncol = 4)
m2 <- matrix(2:13, ncol = 4)
m3 <- matrix(c(2:10, 1:7), ncol = 4)

rownames(m1) <- 1:3
rownames(m2) <- 2:4
rownames(m3) <- 2:5

mat_list <- list(
    m1, m2, m3
)
tpcaObj <- new("tpcaResult", ObjList = mat_list)
SetContrastDistMat(tpcaObj, matrix(c(0, 1, 0, 1), ncol = 2))
```

SetCtrlCondName,tpcaResult-method
Set CtrlCondName

Description

Set CtrlCondName

Usage

```
## S4 method for signature 'tpcaResult'
SetCtrlCondName(object, name)
```

Arguments

object	an object of class tpcaResult
name	a character string describing the control condition

Value

an object of class tpcaResult

Examples

```
tpcaObj <- new("tpcaResult")
SetCtrlCondName(tpcaObj, "DMSO")
```

SetDiffTpcaResultTable,tpcaResult-method
Set diffTpcaResultTable

Description

Set diffTpcaResultTable

Usage

```
## S4 method for signature 'tpcaResult'
SetDiffTpcaResultTable(object, df)
```

Arguments

object	an object of class tpcaResult
df	a data frame containing the results from a differential tpca analysis

Value

an object of class tpcaResult

Examples

```
m1 <- matrix(1:12, ncol = 4)
m2 <- matrix(2:13, ncol = 4)
m3 <- matrix(c(2:10, 1:7), ncol = 4)

rownames(m1) <- 1:3
rownames(m2) <- 2:4
rownames(m3) <- 2:5

mat_list <- list(
    m1, m2, m3
)
tpcaObj <- new("tpcaResult", ObjList = mat_list)
SetDiffTpcaResultTable(tpcaObj, data.frame(pair = "A:B"))
```

SetDistMat,tpcaResult-method
Set DistMat

Description

Set DistMat

Usage

```
## S4 method for signature 'tpcaResult'
SetDistMat(object, mat)
```

Arguments

object	an object of class tpcaResult
mat	matrix containg distance matrix to set

Value

a data frame containing the results from a tpca analysis

Examples

```
m1 <- matrix(1:12, ncol = 4)
m2 <- matrix(2:13, ncol = 4)
m3 <- matrix(c(2:10, 1:7), ncol = 4)

rownames(m1) <- 1:3
rownames(m2) <- 2:4
rownames(m3) <- 2:5

mat_list <- list(
    m1, m2, m3
)
tpcaObj <- new("tpcaResult", ObjList = mat_list)
SetDistMat(tpcaObj, matrix(c(0, 1, 0, 1), ncol = 2))
```

SetDistMethod,tpcaResult-method
Set distMethod

Description

Set distMethod

Usage

```
## S4 method for signature 'tpcaResult'
SetDistMethod(object, method)
```

Arguments

object	an object of class tpcaResult
method	character string of dist method

Value

an object of class tpcaResult

Examples

```
tpcaObj <- new("tpcaResult")
SetDistMethod(tpcaObj, "euclidean")
```

SetPPiRocTable,tpcaResult-method
Set PPiRocTable

Description

Set PPiRocTable

Usage

```
## S4 method for signature 'tpcaResult'
SetPPiRocTable(object, df)
```

Arguments

object	an object of class tpcaResult
df	data.frame containg PPiRocTable to set

Value

an object of class tpcaResult

Examples

```
m1 <- matrix(1:12, ncol = 4)
m2 <- matrix(2:13, ncol = 4)
m3 <- matrix(c(2:10, 1:7), ncol = 4)

rownames(m1) <- 1:3
rownames(m2) <- 2:4
rownames(m3) <- 2:5

mat_list <- list(
    m1, m2, m3
)
tpcaObj <- new("tpcaResult", ObjList = mat_list)
SetPPiRocTable(tpcaObj, data.frame(FPR = 1, TPR = 1))
```

SetPPiRocTableAnno,tpcaResult-method
Set PPiRocTableAnno

Description

Set PPiRocTableAnno

Usage

```
## S4 method for signature 'tpcaResult'
SetPPiRocTableAnno(object, df)
```

Arguments

object	an object of class tpcaResult
df	data.frame containg PPiRocTable annotation to set

Value

an object of class tpcaResult

Examples

```
m1 <- matrix(1:12, ncol = 4)
m2 <- matrix(2:13, ncol = 4)
m3 <- matrix(c(2:10, 1:7), ncol = 4)

rownames(m1) <- 1:3
rownames(m2) <- 2:4
rownames(m3) <- 2:5

mat_list <- list(
    m1, m2, m3
)
tpcaObj <- new("tpcaResult", ObjList = mat_list)
SetPPiRocTableAnno(tpcaObj, data.frame(pair = "A:B"))
```

SetSummaryMethod,tpcaResult-method
Set summaryMethod

Description

Set summaryMethod

Usage

```
## S4 method for signature 'tpcaResult'
SetSummaryMethod(object, method)
```

Arguments

object	an object of class tpcaResult
method	character string of summary method

Value

an object of class tpcaResult

Examples

```
tpcaObj <- new("tpcaResult")
SetSummaryMethod(tpcaObj, "median")
```

SetTpcaResultTable,tpcaResult-method
Set TpcaResultTable

Description

Set TpcaResultTable

Usage

```
## S4 method for signature 'tpcaResult'
SetTpcaResultTable(object, df)
```

Arguments

object	an object of class tpcaResult
df	a data frame containing the results from a tpca analysis

Value

an object of class tpcaResult

Examples

```
m1 <- matrix(1:12, ncol = 4)
m2 <- matrix(2:13, ncol = 4)
m3 <- matrix(c(2:10, 1:7), ncol = 4)

rownames(m1) <- 1:3
rownames(m2) <- 2:4
rownames(m3) <- 2:5

mat_list <- list(
    m1, m2, m3
)
tpcaObj <- new("tpcaResult", ObjList = mat_list)
SetTpcaResultTable(tpcaObj, data.frame(pair = "A:B"))
```

---

string_ppi_df *Data frame of annotated human protein-protein interactions retrieved from stringDB with a combined interaction score equal or higher than 700*

Description

data frame assigning proteins to interacting proteins

Usage

```
data("string_ppi_df")
```

Format

data frame with columns x, y (gene symbol of interactors), combined_score, pair (unique pair id)

References

Jensen et al. (2009), Nucleic Acids Research, 37, D412–D416

Examples

```
data("string_ppi_df")
```

SummaryMethod,tpcaResult-method *Extract SummaryMethod*

Description

Extract SummaryMethod

Usage

```
## S4 method for signature 'tpcaResult'
SummaryMethod(object)
```

Arguments

object	and object of class tpcaResult

Value

a character string of the summary method

Examples

```
tpcaObj <- new("tpcaResult")
SummaryMethod(tpcaObj)
```

---

tpcaResult-class *S4 TPCA Result Class*

Description

S4 TPCA Result Class

Value

an object of class tpcaResult with the following slots: 1) ObjList: containing the supplied list of objects (e.g. a list of Expression Sets summarizing a TPP experiment) 2) ContrastList: containing the supplied list of constrast objects (if supplied for performance of a differential Rtpca analysis) 3) CtrlCondName: character string indicating the control condition, e.g. "control" 4) ContrastCondName: character string indicating the contrast condition, e.g. "drug treatment" 5) DistMat: a matrix containing all pairwise protein-protein distances obtained from comparing their melting curves in the control condition 6) ContrastDistMat: a matrix containing all pairwise protein-protein distances obtained from comparing their melting curves in the contrast condition 7) CommonFeatures: a vector containing the features (proteins) found in common between control and contrast condition 8) ComplexAnnotation: a data frame supplied by the user annotating protein to protein complexes 9) ComplexBackgroundDistributionList: a list of distances drawn for random groups of proteins with different number of members 10) PPiAnnotation: a data frame supplied by the user annotating protein-protein interactions 11) PPiRocTable: data frame containing false positive rate and true positive rate based on ranking the TPCA analysis results by euclidean distance of melting curves of protein pairs, annotated PPIs are considered true positives 12) PPiRocTableAnno: annotation to PPiRocTable 13) ComplexRocTable: data frame containing false positive rate and true positive rate based on ranking the TPCA analysis results by euclidean distance of melting curves of proteins within annotated complexes, annotated complexes are considered true positives, proteins in randomly permuted complex annotations are considered false positives 14) summaryMethod: character string of summarization method used to summarize data across replicates 15) distMethod: character string of distance method used to compare melting curves of proteins 16) tpcaResultTable: data frame containing the results from a tpca analysis 17) diffTpcaResultTable: data frame containing the results from a differential tpca analysis

Slots

`ObjList` list.

`ContrastList` list.

`CtrlCondName` character.

ContrastCondName character.

DistMat matrix.

ContrastDistMat matrix

CommonFeatures vector.

ComplexAnnotation data.frame.

ComplexBackgroundDistributionList list.

PPiAnnotation data.frame.

PPiRocTable data.frame

PPiRocTableAnno data.frame

ComplexRocTable data.frame

summaryMethod character.

distMethod character.

tpcaResultTable data.frame.

diffTpcaResultTable data.frame.

Examples

```
m1 <- matrix(1:12, ncol = 4)
m2 <- matrix(2:13, ncol = 4)
m3 <- matrix(c(2:10, 1:7), ncol = 4)

rownames(m1) <- 1:3
rownames(m2) <- 2:4
rownames(m3) <- 2:5

mat_list <- list(
    m1, m2, m3
)
tpcaObj <- new("tpcaResult", ObjList = mat_list)
```

---

tpcaResultTable,tpcaResult-method

Extract tpcaResultTable

Description

Extract tpcaResultTable

Usage

```
## S4 method for signature 'tpcaResult'
tpcaResultTable(object)
```

Arguments

object	an object of class tpcaResult

Value

a data frame containing the results from a tpca analysis

Examples

```
m1 <- matrix(1:12, ncol = 4)
m2 <- matrix(2:13, ncol = 4)
m3 <- matrix(c(2:10, 1:7), ncol = 4)

rownames(m1) <- 1:3
rownames(m2) <- 2:4
rownames(m3) <- 2:5

mat_list <- list(
    m1, m2, m3
)
tpcaObj <- new("tpcaResult", ObjList = mat_list)
tpcaResultTable(tpcaObj)
```

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