Package ‘rcellminer’

April 11, 2024

Type Package

Title rcellminer: Molecular Profiles, Drug Response, and Chemical Structures for the NCI-60 Cell Lines

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Description The NCI-60 cancer cell line panel has been used over the course of several decades as an anti-cancer drug screen. This panel was developed as part of the Developmental Therapeutics Program (DTP, http://dtp.nci.nih.gov/) of the U.S. National Cancer Institute (NCI). Thousands of compounds have been tested on the NCI-60, which have been extensively characterized by many platforms for gene and protein expression, copy number, mutation, and others (Reinhold, et al., 2012). The purpose of the CellMiner project (http://discover.nci.nih.gov/cellminer) has been to integrate data from multiple platforms used to analyze the NCI-60 and to provide a powerful suite of tools for exploration of NCI-60 data.

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LazyData true

Imports stringr, gplots, ggplot2, methods, stats, utils, shiny

Depends R (>= 3.2), Biobase, rcellminerData (>= 2.0.0)

Suggests knitr, RColorBrewer, sqldf, BiocGenerics, testthat, BiocStyle, jsonlite, heatmaply, glmnet, foreach, doSNOW, parallel, rmarkdown

URL http://discover.nci.nih.gov/cellminer/

VignetteBuilder knitr

biocViews aCGH, CellBasedAssays, CopyNumberVariation, GeneExpression, Pharmacogenomics, Pharmacogenetics, miRNA, Cheminformatics, Visualization, Software, SystemsBiology

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.onAttach

Display citation message

Description

Display citation message

Usage

.onAttach(libname, pkgname)
Arguments

libname  a character string giving the library directory where the package defining the namespace was found.

pkgname  a character string giving the name of the package.

.onLoad  Make sure that rcellminerData is loaded

Description

Make sure that rcellminerData is loaded

Usage

.onLoad(libname, pkgname)

Arguments

libname  a character string giving the library directory where the package defining the namespace was found.

pkgname  a character string giving the name of the package.

cmVersion  CellMiner Version

Description

CellMiner Version

Details

The version of CellMiner used

Author(s)

Vinodh Rajapakse <vinodh.rajapakse AT nih.gov>

References

http://discover.nci.nih.gov/cellminer
**crossCors**

*Calculate cross-correlations with between rows of input matrices*

**Description**

Calculate cross-correlations with between rows of input matrices

**Usage**

```r
crossCors(X, Y = NULL, method = "pearson")
```

**Arguments**

- **X**: a matrix or data.frame
- **Y**: a matrix or data.frame
- **method**: a string specifying the type of correlation, chosen from pearson (default) or spearman.

**Value**

a list containing matrices of pairwise correlations and their p-values between rows of the input matrices or dataframes.

**Author(s)**

Sudhir Varma, NCI-LMP, with input checks, support for Spearman’s correlation added by VNR.

**Examples**

```r
drugActData <- exprs(getAct(rcellminerData::drugData))
crossCors(drugActData[c("94600"), ], drugActData[c("727625", "670655"), ])
crossCors(drugActData[c("94600"), ], drugActData[c("727625", "670655"), ], method="spearman")
```

---

**crossCorsSpearman**

*Calculate Spearman’s correlations with between rows of input matrices*

**Description**

Calculate Spearman’s correlations with between rows of input matrices

**Usage**

```r
crossCorsSpearman(X, Y = NULL)
```
DrugData

Arguments

X  a matrix or data.frame
Y  a matrix or data.frame

Value

A list containing matrices of pairwise Spearman’s correlations and their p-values between rows of the input matrices or dataframes.

Examples

## Not run:
crossCorsSpearman(drugActData[c("94600"), ], drugActData[c("727625", "670655"), ])
## End(Not run)

DrugData  

Returns a DrugData object.

Description

Returns a DrugData object.

Usage

DrugData(act, repeatAct, sampleData, ...)

Arguments

act  An eSet object containing drug activity data across a set of biological samples.
repeatAct  An eSet object containing repeat drug activity experiment data with respect to the same samples associated with act.
sampleData  A MIAxE object capturing sample and other data set information.
...  Other possible parameters.

Value

A DrugData object.
DrugData, eSet, eSet, MIAxE-method

Returns a DrugData object.

Description

Returns a DrugData object.

Usage

```r
## S4 method for signature 'eSet,eSet,MIAxE'
DrugData(act, repeatAct, sampleData, ...)
```

Arguments

- `act` An eSet object containing drug activity data across a set of biological samples.
- `repeatAct` An eSet object containing repeat drug activity experiment data with respect to the same samples associated with `act`.
- `sampleData` A MIAxE object capturing sample and other data set information.
- `...` Other possible parameters.

Value

A DrugData object.

DrugData-class

An S4 class to represent drug activity and related data recorded for a set of biological samples.

Description

An S4 class to represent drug activity and related data recorded for a set of biological samples.

Arguments

- `...` Other possible parameters.

Slots

- `act` An eSet object containing drug activity data across a set of biological samples.
- `repeatAct` An eSet object containing repeat drug activity experiment data with respect to the same samples associated with `act`.
- `sampleData` A MIAxE object capturing sample and other data set information.
**drugDB**

*CellMiner Drug Response Values*

---

**Description**

CellMiner Drug Response Values

**Details**

A list containing response values and annotations:

- act Z-scores of the averaged negative log GI (growth inhibition) 50 values across repeats for the NCI-60; assay described here: [http://dtp.nci.nih.gov/branches/btb/ivclsp.html](http://dtp.nci.nih.gov/branches/btb/ivclsp.html)
- annot
  - id Dataset identifier; NOTE: DO NOT use this column; the NSC is the primary drug identifier
  - nsc National Service Center identifier; the primary drug identifier
  - name Compound name
  - brand_name Brand name for the compound, if sold commercially
  - formula Compound chemical formula
  - testing_status Information on whether it is known if the compound is FDA approved or undergoing testing in clinical trials
  - source TODO
  - smiles Compound chemical structure as a SMILES string
  - weight Compound chemical weight in g/mol
  - mechanism Pharmacological mechanism of action
  - confidential_flag A flag to indicate if compound information is public
  - total_probes TODO
  - total_good_probes TODO
  - low_correlations TODO
  - failure_reason TODO
  - cas CAS Registry Number; NOTE: Due to data restrictions PubChem IDs are the preferred mapping ID to other datasets
  - pubchem_id PubChem ID

**Author(s)**

Vinodh Rajapakse <vinodh.rajapakse AT nih.gov>

**References**

**Drug_MOA_Key**

A data frame with descriptive information for all compound mechanism of action (MOA) abbreviations used in CellMiner.

**Description**

A data frame with descriptive information for all compound mechanism of action (MOA) abbreviations used in CellMiner.

**elNetMolDataNCI60**

NCI60 Molecular Data

**Description**

Z-scores of values for a variety of assays conducted on the NCI-60 to facilitate comparison. Z-scores calculated over the 60 cell lines for the given feature.

**Details**

A list containing various assay values:

- **cop** Copy number values; Described in Pubmed ID: 24670534
- **exp** Expression values; Obtained from "RNA: 5 Platform Gene Transcript" [http://discover.nci.nih.gov/cellminer/loadDownload.do](http://discover.nci.nih.gov/cellminer/loadDownload.do); Missing values imputed using the R package "impute"
- **mut** Mutation values; Deleterious mutations obtained from TODO
- **pro** Reverse protein lysate array values; Obtain from "Protein: Lysate Array" [http://discover.nci.nih.gov/cellminer/loadDownload.do](http://discover.nci.nih.gov/cellminer/loadDownload.do)
- **mda** NCI-60 metadata.
  - **CNV_GAIN** Proportion of genome copy number gains; Described in Pubmed ID: 24670534
  - **CNV_LOSS** Proportion of genome copy number losses; Described in Pubmed ID: 24670534
  - **CNV_TOTAL** Sum of CNV_GAIN and CNV_LOSS
  - **P53_BIN** Binary TP53 profile curated by William Reinhold
  - **MSI_OGAN_BIN** Binary microsatellite instability (MSI) profile curated by Ogan Abaan using COSMIC data; Obtained from Supplementary Table 1 - Ogan Whole Exome Sequencing (WES) paper in Cancer Res.
  - **EPITHELIAL** Epithelial by tissue of origin - pattern extracted from the CellMiner cell line metadata [http://discover.nci.nih.gov/cellminer/celllineMetadata.do](http://discover.nci.nih.gov/cellminer/celllineMetadata.do)
  - **EPITHELIAL_KURT** Kurt Kohn curation for epithelial-like cell lines based on molecular parameters described in Pubmed ID: 24940735
- **DELETERIOUS** Total deleterious variants from WES dataset; Fabricio Sousa curation
- **MISSENSE** Total missense variants from WES dataset; Fabricio Sousa curation
- **SILENT** Total silent variants from WES dataset; Fabricio Sousa curation
- **TOTAL-AA** Total amino acid changing variants from WES dataset; Fabricio Sousa curation
- **CELL-CELL** Cell-to-cell adhesion curated by William Reinhold
- **DOUBLINGTIME** The doubling time pattern was extracted from the CellMiner cell line metadata [http://discover.nci.nih.gov/cellminer/celllineMetadata.do](http://discover.nci.nih.gov/cellminer/celllineMetadata.do)

**Author(s)**

Vinodh Rajapakse <vinodh.rajapakse AT nih.gov>

**References**

[http://discover.nci.nih.gov/cellminer](http://discover.nci.nih.gov/cellminer)

**fingerprintList**  
*Molecular Fingerprint List*

**Description**

Molecular Fingerprint List

**Author(s)**

Augustin Luna <augustin AT mail.nih.gov>

**References**

[http://discover.nci.nih.gov/cellminer](http://discover.nci.nih.gov/cellminer)

**getAct**  
*Returns an eSet object with drug activity data.*

**Description**

Returns an eSet object with drug activity data.

**Usage**

`getAct(object, ...)`
getAct, DrugData-method

Arguments

object Object for which drug activity data is to be returned.

Value

An eSet object with drug activity data.

description

Returns an eSet object with drug activity data.

Usage

## S4 method for signature 'DrugData'
getAct(object)

Arguments

object DrugData object for which drug activity data is to be returned.

Value

An eSet object with drug activity data.

getActivityRangeStats  Returns a table of activity range statistics for a set of compounds.

Description

Returns a table of activity range statistics for a set of compounds.

Usage

getchActivityRangeStats(
  nscSet,
  concFormat = "NegLogGI50M",
  onlyCellMinerExps = TRUE
)
getAllFeatureData

Arguments

- nscSet: a character vector specifying NSC identifier(s) for compound(s) of interest.
- concFormat: a string selected from "NegLogGI50M" or "IC50MicroM". "NegLogGI50M" specifies activities as the negative log of the 50 inhibitory concentration (molar). "IC50MicroM" specifies activities as the 50 inhibitory concentration (micromolar).
- onlyCellMinerExps: a logical value indicating whether to only return experimental data included in CellMiner (default=TRUE).

Value

a table of activity range statistics for a set of compounds.

Examples

```r
nscSet <- c("609699", "740")
getActivityRangeStats(nscSet)
getActivityRangeStats(nscSet, concFormat="IC50MicroM")
```

getAllFeatureData

Returns a list of feature data matrices.

Description

Returns a list of feature data matrices.

Usage

```r
getAllFeatureData(object, ...)
```

Arguments

- object: Object for which a list of feature data matrices is to be returned.
- ...: Other possible parameters.

Value

A list of feature data matrices.
getAllFeatureData, MolData-method

Returns a list of feature data matrices.

Description

Returns a list of feature data matrices.

Usage

## S4 method for signature 'MolData'
getAllFeatureData(object)

Arguments

object MolData object for which a list of feature data matrices is to be returned.

Value

A list of feature data matrices.

getBinaryMutationData
Compute a binary gene mutation data matrix from SNP and other mutation event-level data.

Description

Compute a binary gene mutation data matrix from SNP and other mutation event-level data.

Usage

getBinaryMutationData(
  mutInfo, mutData, 
  maxVariantFreq = 0.2,
  maxNormalPopulationFreq = 0.005, 
  maxSiftScore = 0.05, 
  minPolyPhenScore = 0.85
)


Arguments

**mutInfo**
A data frame with the following named columns: Gene, the name of the gene associated with the mutation event; probe.ids, a unique identifier specifying the mutation event; SNP_1000_genome, the frequency of the mutation event in SNP 1000; ESP5400, the frequency of the mutation event in ESP5400; SNP_type, the type of mutation event, chosen from "MISSENSE", "FRAMESHIFT", "NON-FRAMESHIFT", "NONSENSE", "SPLICING"; SIFT_score, the SIFT score; Polyphen_score, the POLYPHEN score. Rownames of mutInfo should be set to probe.ids, i.e., the unique mutation event specifier.

**mutData**
A matrix with event level mutation information, with SNPs, etc. along rows and samples along columns. Rownames of mutData should exactly match those of mutInfo. The i-th row of mutInfo should thus give detailed information for the mutation event with data specified in the i-th row of mutData.

**maxVariantFreq**
The maximum proportion of mutant samples (used to exclude frequently occurring events); default value = 0.2.

**maxNormalPopulationFreq**
The maximum frequency of a mutation in the normal population (used to exclude likely germline variants); default value = 0.005.

**maxSiftScore**
The maximum accepted SIFT score (used to exclude presumed non-deleterious mutations); default value = 0.05.

**minPolyPhenScore**
The minimum accepted POLYPHEN score (used to exclude presumed non-deleterious mutations); default value = 0.85.

Value

A binary gene mutation matrix, with genes along rows, samples along columns, and 1s indicating deleterious mutations.

**getColumnQuantiles**

_Calculate quantile for the columns in a matrix_

Description

Calculate quantile for the columns in a matrix

Usage

getColumnQuantiles(X, prob, naRm = FALSE, onlyNonzeroVals = FALSE)

Arguments

**X**
the matrix

**prob**
a numeric probability

**naRm**
a boolean, whether to remove NAs

**onlyNonzeroVals**
a boolean, whether to only include non-zero values
**getDrugActivityData**

**Value**

a vector of quantiles

**Examples**

getColumnQuantiles(matrix(1:25, nrow=5), prob = 0.5)

---

**getDrugActivityData**  
Returns a matrix containing activity (-logGI50) data for a set of compounds.

**Description**

Returns a matrix containing activity (-logGI50) data for a set of compounds.

**Usage**

getDrugActivityData(nscSet, onlyCellMinerExps = TRUE)

**Arguments**

- `nscSet`: A string specifying the NSC identifiers for the compounds.
- `onlyCellMinerExps`: A logical value indicating whether to compute results using only experimental data included in CellMiner (default=TRUE).

**Value**

a matrix with NCI-60 average (over experiments) -logGI50 activity data; compound activity profiles are along rows.

**Examples**

nscSet <- c("141540", "123127") # Etoposide, Doxorubicin.
actData <- getDrugActivityData(nscSet)
getDrugActivityRange  
Returns a vector of log activity range values for set of compounds.

Description

Returns a vector of log activity range values for set of compounds.

Usage

getDrugActivityRange(nscSet, computeIQR = FALSE)

Arguments

nscSet  
a character vector specifying NSC identifier(s) for compound(s) of interest.
computeIQR  
logical value indicated whether inter-quartile range is to be computed; otherwise absolute range is computed (default=FALSE).

Value

a numeric vector of NCI-60 log activity (-logGI50) range values indexed by the identifiers in nscSet.

Examples

nscSet <- c("609699", "740")
getDrugActivityRange(nscSet)

getDrugActivityRepeatData

Returns a matrix containing repeat activity experiment data for a compound.

Description

Returns a matrix containing repeat activity experiment data for a compound.

Usage

getDrugActivityRepeatData(
  nscStr,
  concFormat = "NegLogGI50M",
  onlyCellMinerExps = TRUE
)


getDrugMoaList

Get a list of applicable MOA strings for a drug.

Description
Get a list of applicable MOA strings for a drug.

Usage
getDrugMoaList(nsc, moaToCompoundListMap = NULL)

Arguments

nsc
An NSC string.

moaToCompoundListMap
A named list of character vectors, with each name indicating an MOA class, and its corresponding character vector specifying MOA-associated drugs. If unspecified, this is constructed based on MOA information provided by CellMiner.

Details
LINK TO MOAs?

Value
A character vector giving all MOA classes for the drug.
getDrugName

Get the drug names for a set of NSC identifiers.

Description

Get the drug names for a set of NSC identifiers.

Usage

getDrugName(nscSet)

Arguments

nscSet A character vector of NSC strings

Value

A named character vector indicating the compound names for each NSC in nscSet (with an empty string returned if no such information is available, and an NA returned if the NSC is not included in the CellMiner database).

Examples

nscSet <- c("609699", "94600")
getDrugName(nscSet)

getESetList

Returns a list of eSet objects.

Description

Returns a list of eSet objects.

Usage

getESetList(object, ...)

Arguments

object Object for which a list of eSets is to be returned.
...
Other possible parameters.
getESetList,MolData-method

Value
A list of eSet objects.

Description
Returns a list of eSet objects.

Usage

## S4 method for signature 'MolData'
getESetList(object)

Arguments

object MolData object for which a list of eSet objects is to be returned.

Value
A list of eSet objects.

getFeatureAnnot

Returns a list of data frames with feature information.

Description
Returns a list of data frames with feature information.

Usage

getFeatureAnnot(object, ...)

Arguments

object Object for which feature data is to be returned.
...
Other possible parameters.

Value
A list of data frames with feature information.
getFeatureAnnot, DrugData-method

*Description*

Returns a list of data frames with feature information.

*Usage*

```r
## S4 method for signature 'DrugData'
getFeatureAnnot(object)
```

*Arguments*

- `object`: DrugData object for which feature data is to be returned.

*Value*

A named list of data frames with feature information for drugs and drug repeat experiments.

---

getFeatureAnnot, MolData-method

*Description*

Returns a list of data frames with feature information.

*Usage*

```r
## S4 method for signature 'MolData'
getFeatureAnnot(object)
```

*Arguments*

- `object`: MolData object for which feature data is to be returned.

*Value*

A named list of data frames with feature information for available molecular data types.
getFeatureDataFromMatList

*Extract from a list of matrices the data associated with a set of features.*

**Description**

Extract from a list of matrices the data associated with a set of features.

**Usage**

```r
getFeatureDataFromMatList(
  featureSet,
  dataMatList,
  excludeMissingFeatures = TRUE
)
```

**Arguments**

- `featureSet`: a character vector of feature names.
- `dataMatList`: a list of matrices with feature data organized along the rows, and feature names accessible via `rownames(dataMatList)`.
- `excludeMissingFeatures`: a logical value indicating whether features whose data cannot be found in any matrices in `dataMatList` should be excluded in the output. (default=TRUE).

**Value**

a single matrix containing data for all features in `featureSet`.

**Examples**

```r
featureSet <- c("expSLFN11", "mutSLX4")
molDataMats <- getMolDataMatrices()
featureData <- getFeatureDataFromMatList(featureSet, molDataMats)
```

---

getMedSenLineActivity

*Returns a vector of median sensitive cell line activity (-logGI50) values for a set of compounds.*

**Description**

Returns a vector of median sensitive cell line activity (-logGI50) values for a set of compounds.
Usage

getMedSenLineActivity(
  idSet,
  senLineActZThreshold = 0.5,
  onlyCellMinerExps = TRUE,
  dataSource = "NCI60"
)

Arguments

idSet a character vector specifying identifier(s) for compound(s) of interest.
senLineActZThreshold the minimum activity z-score for a sensitive cell line (default=0.5).
onlyCellMinerExps a logical value indicating whether to base results strictly on experimental data included in CellMiner (default=TRUE).
dataSource character string indicating data source (default="NCI60"). Currently only "NCI60" is supported.

Value

a numeric vector of median sensitive cell line activity (-logGI50) values indexed by the identifiers in idSet.

Examples

idSet <- c("609699", "740")
getMedSenLineActivity(idSet)


getMinDrugActivityRepeatCor

Returns a table indicating, for each compound in a specified set, the least significant correlation and associated p-value between its replicate experiments.

Usage

getMinDrugActivityRepeatCor(nscSet)

Description

Returns a table indicating, for each compound in a specified set, the least significant correlation and associated p-value between its replicate experiments.
getMoaStr

Arguments

nscSet a character vector specifying NSC identifier(s) for compound(s) of interest.

Value

A dataframe containing the following columns: NSC, cor, pval

Examples

nscSet <- c("123528", "339316")
repExpCorTab <- getMinDrugActivityRepeatCor(nscSet)

getMoaStr

Get MOA string

Description

Get MOA string

Usage

getMoaStr(nscStr)

Arguments

nscStr an NSC string

Details

LINK TO MOAs?

Value

A comma-delimited string with MOA

Examples

getMoaStr("94600")
getMoaStr(c("94600", "609699"))
**getMoaToCompounds**

*Get a named list mapping MOA classes to associated compound sets.*

**Description**

Get a named list mapping MOA classes to associated compound sets.

**Usage**

```r
getMoaToCompounds()
```

**Value**

A named list mapping MOA classes to associated compound sets (each represented as a character vector).

**Examples**

```r
moaToCompounds <- getMoaToCompounds()
```

**getMolDataMatrices**

*Returns a list of molecular data type matrices, with rownames in each matrix prefixed with a data type abbreviation.*

**Description**

Returns a list of molecular data type matrices, with rownames in each matrix prefixed with a data type abbreviation.

**Usage**

```r
getMolDataMatrices(molDataMats = NULL)
```

**Arguments**

- `molDataMats` A named list of molecular data type matrices with feature data specified along the rows, and feature names indicated in the row names.

**Value**

A list containing molecular data type matrices, with rownames in each matrix prefixed with a data type abbreviation, e.g., 'exp' for mRNA expression, etc. The matrix-specific data type abbreviations are derived from the names of `molDataMats`. 
getMolDataType

Examples

```r
molDataMats <- getMolDataMatrices()
```

---

getMolDataType

*Get the molecular data type prefixes for a set of features.*

Description

Get the molecular data type prefixes for a set of features.

Usage

```r
getMolDataType(features, prefixLen = 3)
```

Arguments

- `features`: A vector of features.
- `prefixLen`: The length of the molecular data type prefix.

Value

A character vector of molecular data type prefixes.

```r
#' @examples getMolDataType(c("expTP53", "copMDM2", "mutCHEK2", "mutBRAF"))
```

---

getNumDrugActivityRepeats

*Returns a vector indicating the number of drug activity repeat experiments with available data for each member of a set of compounds.*

Description

Returns a vector indicating the number of drug activity repeat experiments with available data for each member of a set of compounds.

Usage

```r
getNumDrugActivityRepeats(nscSet, onlyCellMinerExps = TRUE)
```

Arguments

- `nscSet`: a character vector specifying NSC identifier(s) for compound(s) of interest.
- `onlyCellMinerExps`: a logical value indicating whether to return only the number of experiments with data included in CellMiner (default=TRUE).
getNumMissingLines

Returns a vector indicating the number of NCI-60 cell lines with missing activity data for set of compounds.

Description

Returns a vector indicating the number of NCI-60 cell lines with missing activity data for set of compounds.

Usage

getNumMissingLines(nscSet)

Arguments
	nscSet

a character vector specifying NSC identifier(s) for compound(s) of interest.

Value

a numeric vector indicating the number of NCI-60 cell lines with missing activity data, indexed by the identifiers in nscSet.

Examples

nscSet <- c("1", "17", "89", "609699")
getNumMissingLines(nscSet)
getRepeatAct

Description

Returns an eSet object with drug repeat activity experiment data.

Usage

getRepeatAct(object, ...)

Arguments

object Object for which drug repeat activity experiment data is to be returned.
...
Other possible parameters.

Value

An eSet object with drug repeat activity experiment data.

getRepeatAct,DrugData-method

Returns an eSet object with drug repeat activity experiment data.

Description

Returns an eSet object with drug repeat activity experiment data.

Usage

## S4 method for signature 'DrugData'
getRepeatAct(object)

Arguments

object DrugData object for which drug repeat activity experiment data is to be returned.

Value

An eSet object with drug repeat activity experiment data.
getRsd

Computes the relative standard deviation values with respect to the columns of a matrix or data.frame.

Description
Computes the relative standard deviation values with respect to the columns of a matrix or data.frame.

Usage
getRsd(dat, onlyReturnMedian = TRUE)

Arguments
- dat: a matrix or data.frame with numeric values.
- onlyReturnMedian: a logical value indicating whether only the median column RSD value should be returned (vs. all RSD values).

Value
median RSD value over the data set columns or all RSD values, depending on value of onlyReturnMedian (default=TRUE).

Examples
A <- matrix(rnorm(10*60), nrow=10)
getRsd(A)
getRsd(A, onlyReturnMedian=FALSE)

getSampleData

Returns a data frame with sample information.

Description
Returns a data frame with sample information.

Usage
getSampleData(object, ...)

Arguments
- object: Object for which sample data is to be returned.
- ...: Other possible parameters.
**getSampleData,DrugData-method**

Returns a data frame with sample information.

**Description**

Returns a data frame with sample information.

**Usage**

```r
## S4 method for signature 'DrugData'
getSampleData(object)
```

**Arguments**

- `object` DrugData object for which sample data is to be returned.

**Value**

A data frame with sample information.

---

**getSampleData,MolData-method**

Returns a data frame with sample information.

**Description**

Returns a data frame with sample information.

**Usage**

```r
## S4 method for signature 'MolData'
getSampleData(object)
```

**Arguments**

- `object` MolData object for which sample data is to be returned.

**Value**

A data frame with sample information.
getSmiles

Get the SMILES strings for a set of NSC identifiers.

Description
Get the SMILES strings for a set of NSC identifiers.

Usage
getSmiles(nscSet)

Arguments
nscSet A character vector of NSC strings

Value
A named character vector indicating the SMILES string for each NSC in nscSet (or NA if no structural information is available).

Examples
nscSet <- c("609699", "94600")
getSmiles(nscSet)

hasMoa

Check if NSC has Mechanism of Action (MOA) Annotation

Description
Check if NSC has Mechanism of Action (MOA) Annotation

Usage
hasMoa(nsc)

Arguments
nsc a string, an NSC identifier

Value
a boolean whether the NSC has an MOA

Examples
hasMoa("754365")
initialize,DrugData-method

Returns a DrugData object.

Description

Returns a DrugData object.

Usage

## S4 method for signature 'DrugData'
initialize(.Object, act, repeatAct, sampleData)

Arguments

/Object/ An object: see "new()" documentation in "methods" package.
act An eSet object containing drug activity data across a set of biological samples.
repeatAct An eSet object containing repeat drug activity experiment data with respect to the same samples associated with act.
sampleData A MIAxE object capturing sample and other data set information.

Value

A DrugData object.

Note

 Seems to be required for definition of a constructor.

initialize,MolData-method

Returns a MolData object.

Description

Returns a MolData object.

Usage

## S4 method for signature 'MolData'
initialize(.Object, eSetList, sampleData)
isPublic

Arguments

- eSetList: A list of eSet objects for a common set of samples.
- sampleData: A MIAxE object capturing sample and other data set information.

Value

A MolData object.

Description

Check if an NSC ID is public

Usage

isPublic(nscs)

Arguments

- nscs: a vector of NSC string IDs

Value

a vector of boolean values of whether each NSC is public

Examples

isPublic("-1")

isPublic(c("-1", "609699"))
**loadCellminerPlotInfo**  
*Returns data to plot CellMiner plots*

**Description**

Returns data to plot CellMiner plots

**Usage**

```r
loadCellminerPlotInfo(returnDf = FALSE)
```

**Arguments**

- `returnDf`: a boolean if a data.frame with all information (default: FALSE)

**Value**

a vector of colors as strings or a data.frame with `dataType`, `label`, `xMin`, `xMax`

**Examples**

```r
loadCellminerPlotInfo()
```

---

**loadNciColorSet**  
*Returns a 60-element color set that matches the color set used on http://discover.nci.nih.gov/*

**Description**

Returns a 60-element color set that matches the color set used on http://discover.nci.nih.gov/

**Usage**

```r
loadNciColorSet(returnDf = FALSE)
```

**Arguments**

- `returnDf`: a boolean if a data.frame with tissue names and abbreviations should be returned (default: FALSE)

**Value**

a vector of colors as strings or a data.frame with tissues, tissue abbreviations, cell line abbreviations and colors
Examples

loadNciColorSet()

MolData

Returns a MolData object.

Description

Returns a MolData object.

Usage

MolData(eSetList, sampleData, ...)

Arguments

eSetList A list of eSet objects for a common set of samples.
sampleData A MIAXE object capturing sample and other data set information.
... Other possible parameters.

Value

A MolData object.

MolData,list,MIAXE-method

Returns a MolData object.

Description

Returns a MolData object.

Usage

## S4 method for signature 'list,MIAXE'
MolData(eSetList, sampleData, ...)

Arguments

eSetList A list of eSet objects for a common set of samples.
sampleData A MIAXE object capturing sample and other data set information.
... Other possible parameters.

Value

A MolData object.
MolData-class

An S4 class to represent molecular data recorded for a set of biological samples.

Description

An S4 class to represent molecular data recorded for a set of biological samples.

Arguments

... Other possible parameters.

Slots

eSetList A list of eSet objects for a common set of samples.
sampleData A MIAxE object capturing sample and other data set information.

parCorPatternComparison

Compare an input pattern against a set of patterns, excluding the predictive effect of a fixed pattern or set of patterns.

Description

Compare an input pattern against a set of patterns, excluding the predictive effect of a fixed pattern or set of patterns.

Usage

parCorPatternComparison(x, Y, Z, updateProgress = NULL)

Arguments

x An N element input pattern specified as either a vector or a 1 x N matrix or data frame.
Y An N element pattern specified as a vector for comparison with the input pattern x or a k x N matrix with k patterns for comparison with the input pattern x specified along the rows, with rownames set appropriately.
Z An N element pattern specified as a vector or a k x N matrix of patterns specified along the rows. These are the patterns whose effect (with respect to a linear model) is to be excluded when comparing x with Y or each row entry of Y. Note that for the partial correlation to be value, the pattern(s) in Z should not overlap with those in x or Y.
updateProgress A optional function to be invoked with each computed partial correlation to indicate progress.
patternComparison

Value

A data frame with pattern comparison results (ordered by PARCOR): NAME: Name of entry in Y being compared. PARCOR: Partial correlation between x and the entry in Y with respect to Z. PVAL: p-value.

Examples

```r
x <- exprs(getAct(rcellminerData::drugData))[["609699", ]
Y <- rcellminer::getAllFeatureData(rcellminerData::molData)[["exp"]][1:100, ]
Z <- rcellminer::getAllFeatureData(rcellminerData::molData)[["exp"]][c("SLFN11", "JAG1"), ]
results <- parCorPatternComparison(x, Y, Z)
Y <- rcellminer::getAllFeatureData(rcellminerData::molData)[["exp"]][1, , drop=TRUE]
Z <- rcellminer::getAllFeatureData(rcellminerData::molData)[["exp"]]["SLFN11", , drop=TRUE]
results <- parCorPatternComparison(x, Y, Z)
```

---

patternComparison  
*Compare an input pattern against a set of patterns.*

Description

Compare an input pattern against a set of patterns.

Usage

```r
patternComparison(pattern, profileMatrixList, method = "pearson")
```

Arguments

- `pattern`: An N element input pattern specified as either a named vector or an 1 x N matrix or data frame. Names (or column names) must match the column names of each element of profileMatrixList.
- `profileMatrixList`: A single matrix (or data frame) or a list of matrices (or data frames). Each matrix (data frame) must be k x N - that is the k patterns for comparison with the input pattern must be specified along the rows, with rownames set appropriately.
- `method`: a string specifying the type of correlation, chosen from pearson (default) or spearman.

Value

A data frame with pattern comparison results. Specifically, if M is the total number patterns in profileMatrixList elements, an M x 2 matrix is returned with sorted Pearson's correlations in the first column and corresponding p-values in the second column. Comparison pattern names are indicated in the row names.
Examples

```r
drugAct <- exprs(getAct(rcellminerData::drugData))
molDataMats <- getMolDataMatrices()[c("exp", "mut")]
molDataMats <- lapply(molDataMats, function(X) X[1:10, ])
pcResults <- patternComparison(drugAct["609699", ], molDataMats)
pcResults <- patternComparison(drugAct["609699", ], molDataMats, method="spearman")
pcResults <- patternComparison(drugAct["609699", ], molDataMats$exp, method="spearman")
```

---

**plotCellMiner**  
*Description: Produces CellMiner-like plots in R*

**Description**

Description: Produces CellMiner-like plots in R

**Usage**

```r
plotCellMiner(
  drugAct,  
  molData,  
  plots,  
  nsc = NULL,  
  gene = NULL,  
  features = NULL,  
  sub = NULL,  
  xLimits = NULL,  
  xLabel = NULL,  
  extraPlot = NULL,  
  verbose = FALSE
)
```

**Arguments**

- `drugAct`: a matrix of drug activity values (cell lines as columns, drug entries as rows)
- `molData`: a list of matrices of a molecular
- `plots`: a vector of characters denoting the plots to include and the order (e.g. c("mut", "drug", "cop"). Currently, supported entries mutations (mut), drug activities (drug), copy number variations (cop)
- `nsc`: a string NSC ID that will be plotted when a "drug" entry appears in the plots vector
- `gene`: a string HUGO gene symbol for which the "mut", "cop", or "exp" plots will be produced if in plots vector
features  a vector of strings that provide the full IDs for elements to be plotted (e.g. mutCDK4 for CDK4 mutations). This overwrites the nsc and gene parameters, but is needed in advanced plots that involve data that involves one-to-many relationships (e.g. many entries for a given gene in the exome data) and a gene symbol is ambiguous.

sub  a vector of strings with sub-titles for each plot

xLimits  a 2 number vector with the the minimum and maximum X-axis values (default: -3,3 for Z-scores, 0,1 for binary entries)

xLabel  a string for the default X-axis label

extraPlot  a list containing title, label, and values (numeric vector of length 60); only one extra plot can be included

verbose  a boolean to show debugging information

Value

None

Author(s)

Augustin Luna <augustin AT mail.nih.gov>

Examples

```
drugAct <- exprs(getAct(rcellminerData::drugData))
molData <- getMolDataMatrices()
plots <- c("mut", "drug", "cop", "xai", "pro")
plotCellMiner(drugAct, molData, plots=plots, nsc="94600", gene="CDK4", verbose=FALSE)

plots <- c("mut", "xai", "cop", "cop", "cop", "cop")
plotCellMiner(drugAct, molData, plots=plots, nsc="94600", gene=c("CDK4", "TP53", "BRAF", "GAPDH"), verbose=FALSE)

plotCellMiner(drugAct, molData, plots=NULL, nsc=NULL, features=c("mutCDK4", "xaiCDK4", "exochr1:101704532_G_T", "mda1S_P53_MUT", "mirhsa-miR-22", "proTP53_26_GBL00064"), verbose=FALSE)
```

Description

Make a simple 2d plot using two variables with ggplot2
Usage

```r
plotCellMiner2D(
  df,
  xCol = "x",
  yCol = "y",
  xLabel = xCol,
  yLabel = yCol,
  title = NULL,
  colorPalette = NULL,
  classCol = NULL,
  tooltipCol = NULL,
  showLegend = FALSE,
  showTrendLine = TRUE,
  showTitle = TRUE,
  singleColor = "#0000FF",
  alpha = 1,
  numberColPrefix = "X",
  xLimVal = NULL,
  yLimVal = NULL,
  pointSize = 3
)
```

Arguments

df: a data.frame with at least two columns
xCol: the name of the column in df with the "x" data. See Note
yCol: the name of the column in df with the "y" data. See Note
xLabel: the x plot label
yLabel: the y plot label
title: the plot title, if null the correlation will appear (DEFAULT: NULL)
colorPalette: a named vector with the names classes and value colors (DEFAULT: NULL)
classCol: the name of the column with the classes. Values in column of df must be a factor (DEFAULT: NULL)
tooltipCol: the name of the column used for tooltips when plotted with plotly
showLegend: boolean, whether to show the legend (DEFAULT: FALSE)
showTrendLine: boolean, whether to show the trendline
showTitle: boolean, whether to show the title
singleColor: a color to be used for all points when a color palette is not provided (DEFAULT: blue)
alpha: value from 0-1, where 0 indicates transparent points (DEFAULT: 1, not transparent)
numberColPrefix: a prefix to add to column names that start with a number that causes issues with ggplot (DEFAULT: X)
Plot NCI-60 drug activity profiles for repeat experiments.

**Description**

Plot NCI-60 drug activity profiles for repeat experiments.

**xLimVal**

A two entry vector (min, max) to set the x-axis

**yLimVal**

A two entry vector (min, max) to set the y-axis

**pointSize**

Size of points on plot (DEFAULT: 3)

**Value**

A ggplot object

**Note**

TROUBLESHOOTING NOTES: 1) Avoid ":" in colnames

Uses ggplot aes_string() which uses parse() to turn your text expression into a proper R symbol that can be resolved within the data.frame. Avoid numbers and spaces in

**Author(s)**

Augustin Luna <augustin AT mail.nih.gov>

**Examples**

```r
## Not run:
# Load data
ci60DrugActZ <- exprs(getAct(rcellminerData::drugData))
ci60GeneExpZ <- getAllFeatureData(rcellminerData::molData)[["exp"]]
# Load colors
colorTab <- loadNciColorSet(returnDf=TRUE)
tissueColorTab <- unique(colorTab[, c("tissues", "colors")])
# Merge data
df <- as.data.frame(t(rbind(nci60DrugActZ["94600"], nci60GeneExpZ["SLFN11"],)))
colnames(df) <- c("y", "x")
df <- cbind(df, colorTab)
# Plot data
plotCellMiner2D(df, xCol="x", yCol="y", xLabel="SLFN11", yLabel="94600")
plotCellMiner2D(df, xCol="x", yCol="y", xLabel="SLFN11", yLabel="94600", showTrendLine = FALSE, showTitle = FALSE)
plotCellMiner2D(df, xCol="x", yCol="y", showTrendLine = FALSE, showLegend = FALSE)
## End(Not run)
```
Usage

```r
plotDrugActivityRepeats(
    nscStr,
    useZScore = FALSE,
    maxRepNum = 5,
    pdfFilename = NULL,
    pdfWidth = 12,
    pdfHeight = 6
)
```

Arguments

- `nscStr`: a string specifying the NSC identifier for a compound.
- `useZScore`: a boolean specifying whether to plot z-transformed data (as opposed to -logGI50 values).
- `maxRepNum`: an integer specifying the maximum number of repeat experiments to plot.
- `pdfFilename`: name of a PDF output
- `pdfWidth`: width of the PDF (default: 12)
- `pdfHeight`: width of the PDF (default: 6)

Value

NONE

Examples

```r
plotDrugActivityRepeats("609699")
plotDrugActivityRepeats("609699", useZScore=TRUE, maxRepNum=3)
```

---

### plotDrugSets

**Produces a barplot of the average values for a set of NSCs with a error bar (one standard deviation)**

Description

Produces a barplot of the average values for a set of NSCs with a error bar (one standard deviation)

Usage

```r
plotDrugSets(
    drugAct,
    drugs,
    mainLabel = "",
    pdfFilename = NULL,
    statistic = "mean"
)
```
**Arguments**

- **drugAct**: a matrix of drug activity values (cell lines as columns, drug entries as rows)
- **drugs**: a vector of NSC IDs whose values will be averaged by cell line
- **mainLabel**: a main label for the plot
- **pdfFilename**: a string file name for a PDF plot, no file output will be produced if this is not provided
- **statistic**: a string, either 'mean' or 'median' (Default: mean)

**Value**

- no values are returned

**Examples**

```r
drugAct <- exprs(getAct(rcellminerData::drugData))
drugs <- rownames(drugAct)[1:8]
plotDrugSets(drugAct, drugs, "Test")
```

---

**removeMolDataType**

Remove molecular data type prefixes from features.

**Description**

Remove molecular data type prefixes from features.

**Usage**

```r
removeMolDataType(features, prefixLen = 3)
```

**Arguments**

- **features**: A vector of features.
- **prefixLen**: The length of the molecular data type prefix.

**Details**

This function is primarily used to remove prefixes from elastic net features.

**Value**

A named vector of features without molecular data type prefixes.

**Examples**

```r
removeMolDataType(c("expTP53", "copMDM2", "mutCHEK2", "mutBRAF"))
```
restrictFeatureMat

Restricts a feature matrix to only include features associated with a specified gene set.

Description

Restricts a feature matrix to only include features associated with a specified gene set.

Usage

`restrictFeatureMat(geneSet, featureMat, prefixSet = c("cop", "exp", "mut"))`

Arguments

- `featureMat`: a matrix or data frame with feature vectors along rows and feature names specified in `rownames(featureMat)`.
- `prefixSet`: a set of feature name prefixes to be prepended to each element of `geneSet` to obtain a collection of `geneSet`-associated features.

Value

A matrix containing the features in the intersection of `rownames(featureMat)` and the set of `geneSet`-derived features (obtained by prepending each element of `prefixSet` to each gene in `geneSet`).

```r
# Example
X <- matrix(1:25, nrow=5) rownames(X) <- c("expA", "expB", "copC", "mutC", "expD") restrictFeatureMat(geneSet = c("B", "C"), X)
```

rowCors

Row-wise correlations

Description

Correlation between ith row of x and ith row of y for all i

Usage

`rowCors(X, Y)`

Arguments

- `X`: a matrix
- `Y`: a matrix

Value

A list of two vectors: `cor` (correlation values) and `pval` (correlation p-values)
Author(s)

Sudhir Varma, NCI-LMP

Examples

```r
a <- matrix(runif(100), nrow=10, ncol=10)
b <- matrix(runif(100), nrow=10, ncol=10)
c <- rowCors(a, b)
```

Description

Search for NSCs

Usage

```r
searchForNsCs(pattern)
```

Arguments

- `pattern` a search pattern. This string will be treated as a regular expression with the case ignored.

Details

Use this function with caution. Not all compounds have names and compounds can have many synonyms not included in CellMiner.

Value

A vector of matching NSCs

Examples

```r
searchForNsCs("nib$")
```
selectCorrelatedRows  Select features that are correlated with a given feature (or one or more features from a set of features).

Description
Select features that are correlated with a given feature (or one or more features from a set of features).

Usage
selectCorrelatedRows(Y, X, corThreshold = 0.1, useAbsCor = TRUE)

Arguments
Y  a vector or matrix; rows from X will be correlated with Y if Y is a vector or with rows of Y, if Y is a matrix.
X  a matrix of values that will be compared with Y (vector) or rows of Y (matrix)
corThreshold  the minimum correlation threshold for the row to be returned
useAbsCor  a logical value indicating whether absolute correlations should be used (default=TRUE).

Value
a matrix of rows of X correlated with Y (if Y is a vector) or correlated with at least one row of Y if Y is a matrix or data frame.

Examples
vec <- runif(10)
mat <- matrix(runif(100), 10, 10)
selectCorrelatedRows(vec, mat)

selectCorrelatedRowsFromMatrices
Select features that are correlated with a given feature (or one or more features from a set of features), merging results from multiple candidate feature matrices.

Description
Select features that are correlated with a given feature (or one or more features from a set of features), merging results from multiple candidate feature matrices.
Usage

selectCorrelatedRowsFromMatrices(
    Y,
    XList,
    corThreshold = 0.1,
    useAbsCor = TRUE
)

Arguments

Y             a vector or matrix; rows from each matrix element of X will be correlated with
              Y if Y is a vector or with rows of Y, if Y is a matrix.
XList         a list of matrices whose rows will be correlated with Y (vector) or rows of Y
              (matrix). The rownames in each matrix element of XList must be specified to
              values that are unique with respect to the total set of rownames (as derived from
              all matrices in XList).

Value

a matrix formed from rows of matrices in XList that are correlated with Y (if Y is a vector) or
correlated with at least one row of Y if Y is a matrix or data frame.

Examples

vec <- runif(10)
names(vec) <- 1:10
matList <- list(X1 = matrix(runif(100), 10, 10), X2 = matrix(runif(100), 10, 10))
rownames(matList$X1) <- paste0("X1_row_", 1:10)
colnames(matList$X1) <- paste0("X1_col_", 1:10)
rownames(matList$X2) <- paste0("X2_row_", 1:10)
colnames(matList$X2) <- paste0("X2_col_", 1:10)
selectCorrelatedRowsFromMatrices(vec, matList)

[[,MolData-method

Returns an indexed eSet object from a MolData object eSet list.

Description

Returns an indexed eSet object from a MolData object eSet list.

Usage

## S4 method for signature 'MolData'
x[[i]]
Arguments

x A MolData object.
i Index or named item in MolData object eSet list.

Value

An indexed eSet object from a MolData object eSet list.

[[<-,MolData-method

Assigns an eSet object to a specified position in a MolData object eSet list.

Description

Assigns an eSet object to a specified position in a MolData object eSet list.

Usage

## S4 replacement method for signature 'MolData'
x[[i]] <- value

Arguments

x A MolData object.
i Index or named item in MolData object eSet list.
value An eSet object to be assigned.

Value

An eSet object to a specified position in a MolData object eSet list.
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