Package ‘ToxicoGx’

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Description

The function fetches a table of all ToxicoSets available for download from the ToxicoGx server. The table includes the names of the ToxicoSet, the types of data available in the object, and the date of last update.

Usage

availableTSets(canonical = TRUE)

Arguments

canonical logical Should available TSets show only official TSets, or should user generated TSets be included?

Details

Much more information on the processing of the data and data provenance can be found at: www.orcestra.ca

Value

A data.frame with details about the available ToxicoSet objects

Examples

if (interactive()){ availableTSets() }
checkTSetStructure  

*Function to verify the structure of a ToxicoSet*

**Description**

This function checks the structure of a ToxicoSet, ensuring that the correct annotations are in place and all the required slots are filled so that matching of cells and drugs can be properly done across different types of data and with other studies.

**Usage**

```r
checkTSetStructure(tSet, plotDist = FALSE, result.dir = ".")
```

**Arguments**

- **tSet**: A ToxicoSet object
- **plotDist**: Should the function also plot the distribution of molecular data?
- **result.dir**: The path to the directory for saving the plots as a string, defaults to `tempdir()`

**Value**

Prints out messages whenever describing the errors found in the structure of the pset object passed in.

**Examples**

```r
checkTSetStructure(TGGATESTsmall)
```

---

**computeAUC**

*Computes the AUC for a Drug Dose Viability Curve*

**Description**

Returns the AUC (Area Under the drug response Curve) given concentration and viability as input, normalized by the concentration range of the experiment. The area returned is the response (1-Viability) area, i.e. area under the curve when the response curve is plotted on a log10 concentration scale, with high AUC implying high sensitivity to the drug. The function can calculate both the area under a fitted Hill Curve to the data, and a trapz numeric integral of the actual data provided. Alternatively, the parameters of a Hill Slope returned by logLogisticRegression can be passed in if they already known.
computeAUC

Usage

computeAUC(
  concentration,
  viability,
  Hill_fit,
  conc_as_log = FALSE,
  viability_as_pct = TRUE,
  trunc = TRUE,
  area.type = c("Fitted", "Actual"),
  verbose = TRUE
)

Arguments

collection vector is a vector of drug concentrations.

viability vector is a vector whose entries are the viability values observed in the presence of the drug concentrations whose logarithms are in the corresponding entries of conc, where viability 0 indicates that all cells died, and viability 1 indicates that the drug had no effect on the cells.

Hill_fit list or vector In the order: c("Hill Slope", "E_inf", "EC50"), the parameters of a Hill Slope as returned by logLogisticRegression. If conc_as_log is set then the function assumes logEC50 is passed in, and if viability_as_pct flag is set, it assumes E_inf is passed in as a percent. Otherwise, E_inf is assumed to be a decimal, and EC50 as a concentration.

conc_as_log logical, if true, assumes that log10-concentration data has been given rather than concentration data.

viability_as_pct logical, if false, assumes that viability is given as a decimal rather than a percentage, and returns AUC as a decimal. Otherwise, viability is interpreted as percent, and AUC is returned 0-100.

trunc logical, if true, causes viability data to be truncated to lie between 0 and 1 before curve-fitting is performed.

area.type Should the area be computed using the actual data ("Actual"), or a fitted curve ("Fitted")

verbose logical, if true, causes warnings thrown by the function to be printed.

Value

Numeric AUC value

Examples

dose <- c("0.0025","0.008","0.025","0.08","0.25","0.8","2.53","8")
viability <- c("108.67","111","102.16","100.27","90","87","74","57")
computeAUC(dose, viability)
computeIC50  

Computes the ICn for any n in 0-100 for a Drug Dose Viability Curve

Description

Returns the ICn for any given nth percentile when given concentration and viability as input, normalized by the concentration range of the experiment. A Hill Slope is first fit to the data, and the ICn is inferred from the fitted curve. Alternatively, the parameters of a Hill Slope returned by logLogisticRegression can be passed in if they already known.

Usage

```r
computeIC50(
  concentration,
  viability,
  Hill_fit,
  conc_as_log = FALSE,
  viability_as_pct = TRUE,
  verbose = TRUE,
  trunc = TRUE
)
```

```r
computeICn(
  concentration,
  viability,
  Hill_fit,
  n,
  conc_as_log = FALSE,
  viability_as_pct = TRUE,
  verbose = TRUE,
  trunc = TRUE
)
```

Arguments

- **concentration** vector is a vector of drug concentrations.
- **viability** vector is a vector whose entries are the viability values observed in the presence of the drug concentrations whose logarithms are in the corresponding entries of conc, where viability 0 indicates that all cells died, and viability 1 indicates that the drug had no effect on the cells.
- **Hill_fit** list or vector In the order: c("Hill Slope", "E_inf", "EC50"), the parameters of a Hill Slope as returned by logLogisticRegression. If conc_as_log is set then the function assumes logEC50 is passed in, and if viability_as_pct flag is set, it assumes E_inf is passed in as a percent. Otherwise, E_inf is assumed to be a decimal, and EC50 as a concentration.
- **conc_as_log** logical, if true, assumes that log10-concentration data has been given rather than concentration data, and that log10(ICn) should be returned instead of ICn.
viability_as_pct
  logical, if false, assumes that viability is given as a decimal rather than a percentage, and that E_inf passed in as decimal.

verbose
  logical, if true, causes warnings thrown by the function to be printed.

trunc
  logical, if true, causes viability data to be truncated to lie between 0 and 1 before curve-fitting is performed.

n
  numeric The percentile concentration to compute. If viability_as_pct set, assumed to be percentage, otherwise assumed to be a decimal value.

Value
  a numeric value for the concentration of the nth percentile viability reduction

Functions
  • computeIC50(): Returns the IC50 of a Drug Dose response curve

Examples
  
dose <- c("0.0025","0.008","0.025","0.08","0.25","0.8","2.53","8")
viability <- c("108.67","111","102.16","100.27","90","87","74","57")
computeIC50(dose, viability)
computeICn(dose, viability, n=10)
computeLimmaDiffExpr,ToxicoSet-method

Conduct differential expression analysis using the limma R package

Description

WARNING: This function can take a very long time to compute!

Usage

## S4 method for signature 'ToxicoSet'
computeLimmaDiffExpr(object, buildTable = TRUE)

Arguments

- **object**
  - A `ToxicoSet` object with a molecular profile named 'rna'
- **buildTable**
  - `logical` Should the result of the eBayes function from limma be assembled into a data.table containing the result along with the gene, compound and durations names. Default it TRUE, otherwise this function will return the object produced by eBayes.

Value

A `data.table` containing the results the limma differential expression analysis comparing control vs each dose level for each compound within each duration.

Examples

```r
if (interactive()) {
  data(TGGATESsmall)
  analysis <- computeLimmaDiffExpr(TGGATESsmall)
}
```

dim,ToxicoSet-method

Get the dimensions of a ToxicoSet

Description

Get the dimensions of a ToxicoSet

Usage

## S4 method for signature 'ToxicoSet'
dim(x)
downloadTSet

Arguments

- `x` ToxicoSet

Value

A named vector with the number of Cells and Drugs in the ToxicoSet

Examples

```r
data(TGGATExsmall)
dim(TGGATExsmall)
```

Description

This function allows you to download a ToxicoSet object for use with this package. The ToxicoSets have been extensively curated and organised within a ToxicoSet class, enabling use with all the analysis tools provided in ToxicoGx.

Usage

```r
downloadTSet(
  name,
  saveDir = tempdir(),
  tSetFileName = NULL,
  verbose = TRUE,
  timeout = 600
)
```

Arguments

- `name` Character string, the name of the PharmacSet to download.
- `saveDir` Character string with the folder path where the ToxicoSet should be saved. Defaults to './tSets/'. Will create directory if it does not exist.
- `tSetFileName` character string, the file name to save the dataset under
- `verbose` bool Should status messages be printed during download. Defaults to TRUE.
- `timeout` numeric(1) How long to wait before the download times out, in seconds. Default is 600 seconds (10 minutes).

Value

A tSet object with the dataset, downloaded from our server
Examples

```r
if (interactive()) {
  drugMatrix_rat <- downloadTSet("DrugMatrix Rat")
}
```

---

**drugGeneResponseCurve**  
Compares gene expression for a specified set of features over specific drug dosages vs time

---

Description

This function generates a plot visualizing the relationship between gene expression, time and dose level for the selected tSet. The plot is generated with ggplot2 and can be customized using ggplot2 `plot + function()` syntax.

Usage

```r
drugGeneResponseCurve(
  tSet,  
  duration = NULL,  
  cell_lines = NULL,  
  mDataTypes = NULL,  
  features = NULL,  
  dose = NULL,  
  drug = NULL,  
  summarize_replicates = TRUE,  
  line_width = 1,  
  point_size = 2.5,  
  ggplot_args = NULL,  
  verbose = TRUE
)
```

Arguments

- **tSet** ToxicoSet A ToxicoSet to be plotted in this graph. Currently only a single tSet is supported.
- **duration** character A vector of durations to include in the plot.
- **cell_lines** character A vector of cell lines to include in the plot.
- **mDataTypes** vector A vector specifying the molecular data types to include in this plot. Defaults to the first mDataType if not specified. ex This release version only accepts one mDataType, more to be added in forthcoming releases.
- **features** character A vector of feature names to include in the plot. If you specify more than two dose levels, you may only pass in up to two features.
**drugPerturbationSig**

*Drug perturbation analysis*

**Description**

Creates a signature representing gene expression (or other molecular profile) change induced by administrating a drug, for use in drug effect analysis.

**Usage**

```r
drugPerturbationSig(
  tSet,  
mDataType,  
drugs = NULL,  
cell_lines = NULL,
```

---

**dose**

character A vector of dose levels to be included in the plot. Default to include all dose levels available for a drug. If you specify more than two features you may only pass in up to two dose levels.

**drug**

character A drug name to include in this plot. See treatmentNames(tSet) for a list of options.

**summarize_replicates**

logical If TRUE will average viability across replicates for each unique drug-dose-duration combination.

**line_width**

numeric A number specifying the thickness of lines in the plot, as passed to size in geom_line(). Defaults to 1.

**point_size**

numeric A number specifying how large points should be in the plot, as passed to size in geom_point(). Defaults to 2.5.

**ggplot_args**

list A list of ggplot2 functions which can be called using the plot + function() syntax. This allows arbitrary customization of the plot including changing the title, axis labels, colours, etc. Please see the included examples for basic usage or ggplot2 documentation for advanced customization.

**verbose**

boolean Should warning messages about the data passed in be printed?

**Value**

Plot of the viabilities for each drug vs time of exposure

**Examples**

```r
if (interactive()) {
  drugGeneResponseCurve(TGGATESsmall, dose = c("Control", "Low", "Middle"),  
mDataTypes="rna", drug = treatmentNames(TGGATESsmall)[1],  
duration = c("2", "8", "24"), features = "ENSG00000002726_at")
}
```
features = NULL,
duration = NULL,
dose = NULL,
nthread = 1,
returnValues = c("estimate", "tstat", "pvalue", "fdr"),
verbose = FALSE)
}

Arguments
tSet ToxicoSet a ToxicoSet of the perturbation experiment type
mDataType character which one of the molecular data types to use in the analysis, out of dna, rna, rnaseq, snp, cnv (only rna currently supported)
drugs character a vector of drug names for which to compute the signatures. Should match the names used in the ToxicoSet.
cell_lines character a vector of cell names to use in computing the signatures. Should match the names used in the ToxicoSet.
features character a vector of features for which to compute the signatures. Should match the names used in correspondant molecular data in ToxicoSet.
duration character a vector of experiment durations for which to include in the computed the signatures.
dose character a vector of dose levels to include in the results
nthread numeric if multiple cores are available, how many cores should the computation be parallelized over?
returnValues character Which of estimate, t-stat, p-value and fdr should the function return for each gene drug pair
verbose bool Should diagnostic messages be printed? (default false)

Details
Given a Toxicoset of the perturbation experiment type, and a character vector of drugs, the function will compute a signature for the effect of drug concentration on the molecular profile of a cell. The algorithm uses a regression model which corrects for experimental batch effects, cell specific differences, and duration of experiment to isolate the effect of the concentration of the drug applied. The function returns the estimated coefficient for concentration, the t-stat, the p-value and the false discovery rate associated with that coefficient, in a 3 dimensional array, with genes in the first direction, drugs in the second, and the selected return values in the third.

Value
ToxicoSig An object composed of a 3D array with genes in the first dimension, drugs in the second, and return values in the third.
Examples

```r
if (interactive()) {
  data(TGGATESsmall)
  drug.perturbation <- drugPerturbationSig(TGGATESsmall, mDataType="rna", features = head(fNames(TGGATESsmall, "rna"), 10),
  }
```

---

**drugTimeResponseCurve**  
Compares viabilities at a given dose over different experimental durations

---

**Description**

This function generates a plot visualizing the relationship between gene expression, time and dose level for the selected tSet. The plot is generated with ggplot2 and can be customized using ggplot plot + function() syntax.

**Usage**

```r
drugTimeResponseCurve(
  tSet,  
  duration = NULL,
  cell_lines = NULL,
  dose = NULL,
  drugs = NULL,
  summarize_replicates = TRUE,
  line_width = 1,
  point_size = 2.5,
  verbose = TRUE,
  ggplot_args = NULL
)
```

**Arguments**

- **tSet**  
  ToxicoSet  
  A ToxicoSet to be plotted in this figure

- **duration**  
  character  
  A vector of durations to include in the plot.

- **cell_lines**  
  character  
  A vector of cell lines to include in the plot.

- **dose**  
  character  
  A vector of dose levels to be included in the plot. Default to include all dose levels available for a drug. Must include at minimum two dose levels, one of which is "Control".

- **drugs**  
  character  
  A drugs or pair of drugs to be plotted.

- **summarize_replicates**  
  logical  
  If TRUE will average viability across replicates for each unique drug-dose-duration combination.

- **line_width**  
  numeric  
  A number specifying the thickness of lines in the plot, as passed to size in geom_line(). Defaults to 1.
point_size numeric A number specifying how large points should be in the plot, as passed to size in geom_point(). Defaults to 2.5.

verbose boolean Should warning messages about the data passed in be printed?

ggplot_args list A list of ggplot2 functions which can be called using the plot + function() syntax. This allows arbitrary customization of the plot including changing the title, axis labels, colours, etc. Please see the included examples for basic usage or ggplot2 documentation for advanced customization. Alternatively, you could assign the return value to a variable and add the customization yourself using plot + function().

Value

Plot of the viabilities for each drug vs time of exposure

Examples

library(ggplot2)

# Default settings
plot <- drugTimeResponseCurve(TGGATESsmall, cell_lines = "Hepatocyte",
   dose = c("Control", "Low", "Middle"), drugs = treatmentNames(TGGATESsmall)[6],
   duration = c("2", "8", "24"))

# Customize title, x/y labels, x/y limits, colour palette and define
# custom ticks for x axis using the function argument ggplot2_args
customizations <- list(labs(title = 'My Custom Title', ylab = 'The y-axis',
   xlim(c(2, 24)), ylim(c(99,105)),
   scale_color_brewer(palette="Set1"),
   scale_x_continuous(breaks=c(2, 8, 24),
   labels = c("Two", "Eight", "Twenty-Four")))

if(interactive()) {
   drugTimeResponseCurve(TGGATESsmall, cell_lines = "Hepatocyte",
      dose = c("Control", "Low", "Middle"),
      drugs = treatmentNames(TGGATESsmall)[6], duration = c("2", "8", "24"),
      ggplot_args = customizations)
}

# Customize the plot using standard ggplot2 syntax
if(interactive()) {
   plot + labs(title = 'My Custom Title', ylab = 'The y-axis') +
      xlim(c(2, 24)) + ylim(c(99,105)) + scale_color_brewer(palette="Set1")
}
geneDrugPerturbation  

*Compute gene-drug associations*

**Description**

Function computing gene-drug associations from perturbation data

**Usage**

geneDrugPerturbation(x, concentration, type, batch, duration, model = FALSE)

**Arguments**

- **x**  
  numeric Vector of gene expression values

- **concentration**  
  numeric Vector with drug concentrations/doses

- **type**  
  factor Vector of factors specifying the cell lines or type types

- **batch**  
  factor Vector of factors specifying the batch

- **duration**  
  character Vector of measurement times (in hours)

- **model**  
  logical Should the full linear model be returned? Default set to FALSE

**Value**

numeric Vector reporting the effect size (estimate of the coefficient of drug concentration), standard error (se), sample size (n), t statistic, and F statistics and its corresponding p-value

**Examples**

ToxicoGx::drugPerturbationSig(tSet = TGGATESsmall,  
    mDataType="rna",  
    cell_lines="Hepatocyte",  
    duration="24",  
    dose=c("Control", "Low"),  
    drugs=c("Omeprazole", "Isoniazid"),  
    returnValues=c("estimate","tstat", "pvalue", "fdr"),  
    verbose=FALSE)
**HCC_sig**  
*HCC_sig dataset*

**Description**

A dataset containing the gene names associated with the HCC geneset signature

**Usage**

```r
data(HCC_sig)
```

**Format**

character

---

**logLogisticRegression**  
*Fits curves of the form* \( E = E_{\text{inf}} + (1 - E_{\text{inf}})/(1 + (c/EC50)^{HS}) \) *to dose-response data points \((c, E)\) given by the user and returns a vector containing estimates for HS, E_inf, and EC50.*

**Description**

By default, `logLogisticRegression` uses an L-BFGS algorithm to generate the fit. However, if this fails to converge to solution, `logLogisticRegression` samples lattice points throughout the parameter space. It then uses the lattice point with minimal least-squares residual as an initial guess for the optimal parameters, passes this guess to `drm`, and re-attempts the optimization. If this still fails, `logLogisticRegression` uses the PatternSearch algorithm to fit a log-logistic curve to the data.

**Usage**

```r
logLogisticRegression(
  conc,  
  viability,  
  density = c(2, 10, 2),  
  step = 0.5/density,  
  precision = 0.05,  
  lower_bounds = c(0, 0, -6),  
  upper_bounds = c(4, 1, 6),  
  scale = 0.07,  
  family = c("normal", "Cauchy"),  
  median_n = 1,  
  conc_as_log = FALSE,  
  viability_as_pct = TRUE,  
  trunc = TRUE,  
  verbose = FALSE
)
```
Arguments

conc vector is a vector of drug concentrations.

viability vector is a vector whose entries are the viability values observed in the presence of the drug concentrations whose logarithms are in the corresponding entries of the log_conc, where viability 0 indicates that all cells died, and viability 1 indicates that the drug had no effect on the cells.

density vector is a vector of length 3 whose components are the numbers of lattice points per unit length along the HS-, E_inf-, and base-10 logarithm of the EC50-dimensions of the parameter space, respectively.

step vector is a vector of length 3 whose entries are the initial step sizes in the HS, E_inf, and base-10 logarithm of the EC50 dimensions, respectively, for the PatternSearch algorithm.

precision is a positive real number such that when the ratio of current step size to initial step size falls below it, the PatternSearch algorithm terminates. A smaller value will cause LogisticPatternSearch to take longer to complete optimization, but will produce a more accurate estimate for the fitted parameters.

lower_bounds vector is a vector of length 3 whose entries are the lower bounds on the HS, E_inf, and base-10 logarithm of the EC50 parameters, respectively.

upper_bounds vector is a vector of length 3 whose entries are the upper bounds on the HS, E_inf, and base-10 logarithm of the EC50 parameters, respectively.

scale is a positive real number specifying the shape parameter of the Cauchy distribution.

family character, if "cauchy", uses MLE under an assumption of Cauchy-distributed errors instead of sum-of-squared-residuals as the objective function for assessing goodness-of-fit of dose-response curves to the data. Otherwise, if "normal", uses MLE with a gaussian assumption of errors

median_n If the viability points being fit were medians of measurements, they are expected to follow a median of family distribution, which is in general quite different from the case of one measurement. Median_n is the number of measurements the median was taken of. If the measurements are means of values, then both the Normal and the Cauchy distributions are stable, so means of Cauchy or Normal distributed variables are still Cauchy and normal respectively.

conc_as_log logical, if true, assumes that log10-concentration data has been given rather than concentration data, and that log10(EC50) should be returned instead of EC50.

viability_as_pct logical, if false, assumes that viability is given as a decimal rather than a percentage, and that E_inf should be returned as a decimal rather than a percentage.

trunc logical, if true, causes viability data to be truncated to lie between 0 and 1 before curve-fitting is performed.

verbose logical, if true, causes warnings thrown by the function to be printed.

Value

A vector containing estimates for HS, E_inf, and EC50
Examples

dose <- c("0.0025","0.008","0.025","0.08","0.25","0.8","2.53","8")
viability <- c("108.67","111","102.16","100.27","90","87","74","57")
computeAUC(dose, viability)

---

show,ToxicoSet-method  Show a ToxicoSet

Description

Show a ToxicoSet

Usage

## S4 method for signature 'ToxicoSet'
show(object)

Arguments

object  A ToxicoSet object to print a summary for

Value

Prints the ToxicoSet object to the output stream, and returns invisible NULL.

Examples

TGGATESsmall

---

show,ToxicoSig-method  Show ToxicoGx Signatures

Description

Show ToxicoGx Signatures

Usage

## S4 method for signature 'ToxicoSig'
show(object)

Arguments

object  ToxicoSig
**showSigAnnot**

**Value**

Prints the ToxicoGx Signatures object to the output stream, and returns invisible NULL.

**Examples**

```r
data(TGGATESsmall)
drug.perturbation <- drugPerturbationSig(TGGATESsmall, mDataType="rna", nthread = 1, duration = "2",
drugs = head(treatmentNames(TGGATESsmall)), features = fNames(TGGATESsmall, "rna")[seq_len(2)])
drug.perturbation
```

---

**showSigAnnot**

*Show the Annotations of a signature object*

**Description**

This function prints out the information about the call used to compute the drug signatures, and the session info for the session in which the computation was done. Useful for determining the exact conditions used to generate signatures.

**Usage**

```
showSigAnnot(Sigs)
```

**Arguments**

- **Sigs**
  
  An object of the ToxicoSig Class, as returned by drugPerturbationSig

**Value**

Prints the ToxicoGx Signatures annotations to the output stream, and returns invisible NULL.

**Examples**

```r
data(TGGATESsmall)
drug.perturbation <- drugPerturbationSig(TGGATESsmall, mDataType="rna", nthread=1, duration = "2",
drugs = head(treatmentNames(TGGATESsmall)), features = fNames(TGGATESsmall, "rna")[seq_len(2)])
showSigAnnot(drug.perturbation)
```
subsetTo

A function to subset a ToxicoSet to data containing only specified drugs, cells and genes

Description

This is the preferred method of subsetting a ToxicoSet. This function allows abstraction of the data to the level of biologically relevant objects: drugs and cells. The function will automatically go through all of the combined data in the ToxicoSet and ensure only the requested radiations and cell lines are found in any of the slots. This allows quickly picking out all the experiments for a radiation or cell of interest, as well removes the need to keep track of all the metadata conventions between different datasets.

Usage

subsetTo(
  object,
  cell_lines = NULL,
  drugs = NULL,
  molecular.data.cells = NULL,
  duration = NULL,
  features = NULL,
  ...
)

Arguments

- **object**  
  A ToxicoSet to be subsettred
- **cell_lines**  
  A list or vector of cell names as used in the dataset to which the object will be subsettred. If left blank, then all cells will be left in the dataset.
- **drugs**  
  A list or vector of drug names as used in the dataset to which the object will be subsettred. If left blank, then all drugs will be left in the dataset.
- **molecular.data.cells**  
  A list or vector of cell names to keep in the molecular data
- **duration**  
  A list or vector of the experimental durations to include in the subset as strings. Defaults to all durations if parameter is not specified.
- **features**  
  A list or vector of feature names as used in the dataset from which the object will be subsettred. If left blank that all features will be left in.
- **...**  
  Other arguments passed to other functions within the package

Value

A ToxicoSet with only the selected drugs and cells
summarizeMolecularProfiles

Examples

```r
tGGATESDrugNames <- treatmentNames(TGGATESsmall)
tGGATESCells <- sampleNames(TGGATESsmall)
tSet <- subsetTo(TGGATESsmall, drugs = TGGATESDrugNames[1],
                    cells = TGGATESCells[1], duration = "2")
```

summarizeMolecularProfiles

Takes molecular data from a ToxicoSet, and summarises them into one
entry per drug and experimental condition.

Description

Given a ToxicoSet with molecular data, this function will summarize the data into one profile per
experimental condition (duration, dose level) using the chosen summary.stat and return a Summa-
rizedExperiment object, with one Assay corresponding to a requested drug.

Usage

```r
summarizeMolecularProfiles(
  tSet,
  mDataType,
  cell_lines = NULL,
  drugs = NULL,
  features = NULL,
  duration = NULL,
  dose = c("Control", "Low", "Middle", "High"),
  summary.stat = c("mean", "median", "first", "last"),
  fill.missing = TRUE,
  summarize = TRUE,
  verbose = TRUE
)
```

Arguments

tSet ToxicoSet The ToxicoSet to summarize
mDataType character which one of the molecular data types to use in the analysis, out of
all the molecular data types available for the tSet for example: rna
cell_lines character The cell lines to be summarized. If any cell.line has no data, missing
values will be created
drugs character The drugs to be summarized
features character A vector of the feature names to include in the summary
duration character A vector of durations to summarize across
dose character The dose level to summarize replicates across
summarizeSensitivityProfiles

summarizeSensitivityProfiles(Takes the sensitivity data from a ToxicoSet, and summarises them into a drug vs cell line table)

Description

This function creates a table with drug as rows and cell lines as columns, summarising the drug sensitivity data of a ToxicoSet into drug-cell line pairs for a specified experiment duration.

Usage

summarizeSensitivityProfiles(
  tSet, duration = NULL, cell_lines = NULL,
Arguments

tSet ToxicoSet The ToxicoSet from which to extract the data
duration numeric The duration at which to summarize the drug-cell combo. This is a required parameter.
cell_lines character The cell lines to be summarized. If any cell lines has no data, it will be filled with missing values
drugs character The drugs to be summarized. If any drugs has no data, it will be filled with missing values. Defaults to include all drugs in the given tSet.
sensitivity.measure character which sensitivity sensitivity.measure to use? Use the sensitivityMeasures function to find out what measures are available for each TSet.
summary.stat character which summary method to use if there are repeated cell line-drug experiments? Choices are "mean", "median", "first", "last", "max", or "min"
fill.missing boolean should the missing cell lines not in the molecular data object be filled in with missing values?
verbose Should the function print progress messages?

Value

matrix A matrix with drugs going down the rows, cell lines across the columns, with the selected sensitivity statistic for each pair.

Examples

data(TGGATESsmall)
TGGATESauc <- summarizeSensitivityProfiles(TGGATESsmall, sensitivity.measure='auc_recomputed')
ToxicoSet

Usage

data(TGGATESsmall)

Format

ToxicoSet object

References


ToxicoSet  ToxicoSet constructor

Description

A constructor that simplifies the process of creating ToxicoSets, as well as creates empty objects for data not provided to the constructor. Only objects returned by this constructor are expected to work with the ToxicoSet methods. For a much more detailed instruction on creating ToxicoSets, please see the "CreatingToxicoSet" vignette.

Usage

ToxicoSet(
  name,
  molecularProfiles = list(),
  sample = data.frame(),
  treatment = data.frame(),
  sensitivityInfo = data.frame(),
  sensitivityRaw = array(dim = c(0, 0, 0)),
  sensitivityProfiles = matrix(),
  sensitivityN = matrix(nrow = 0, ncol = 0),
  perturbationN = array(NA, dim = c(0, 0, 0)),
  curationTreatment = data.frame(),
  curationSample = data.frame(),
  curationTissue = data.frame(),
  datasetType = c("sensitivity", "perturbation", "both"),
  verify = TRUE
)

Arguments

name A character string detailing the name of the dataset
molecularProfiles A list of SummarizedExperiment objects containing molecular profiles for each molecular data type.
**ToxicoSet-accessors**

Accessing and modifying information in a CoreSet

**sample**
A data.frame containing the annotations for all the sample profiled in the dataset, across all data types. Must contain the mandatory `sampleId` column which uniquely identifies each sample in the object.

**treatment**
A data.frame containing annotations for all treatments profiled in the dataset. Must contain the mandatory `treatmentId` column which uniquely identifies each treatment in the object.

**sensitivityInfo**
A data.frame containing the information for the sensitivity experiments. Must contain a 'sampleId' column with unique identifiers to each sample, matching the sample object and a 'treatmentId' columns with unique indentifiers for each treatment, matching the treatment object.

**sensitivityRaw**
A 3 Dimensional array containing the raw drug dose response data for the sensitivity experiments

**sensitivityProfiles**
data.frame containing drug sensitivity profile statistics such as IC50 and AUC

**sensitivityN**, **perturbationN**
A data.frame summarizing the available sensitivity/perturbation data

**curationSample**, **curationTissue**, **curationTreatment**
A data.frame mapping the names for samples, tissues and treatments used in the data set to universal identifiers used between different CoreSet objects

**datasetType**
A character(1) string of 'sensitivity', 'perturbation', or 'both' detailing what type of data can be found in the CoreSet, for proper processing of the data

**verify**
logical(1) Should the function verify the CoreSet and print out any errors it finds after construction?

**Value**

An object of class ToxicoSet

---

**ToxicoSet-accessors**

**Description**

Documentation for the various setters and getters which allow manipulation of data in the slots of a CoreSet object.

**Usage**

```
drugInfo(...)

drugInfo(...) <- value

drugNames(...)
```
drugNames(...) <- value

## S4 method for signature 'ToxicoSet'
annotation(object)

## S4 replacement method for signature 'ToxicoSet,list'
annotation(object) <- value

## S4 method for signature 'ToxicoSet'
dateCreated(object)

## S4 replacement method for signature 'ToxicoSet,character'
dateCreated(object) <- value

## S4 method for signature 'ToxicoSet'
name(object)

## S4 replacement method for signature 'ToxicoSet'
name(object) <- value

## S4 method for signature 'ToxicoSet'
sampleInfo(object)

## S4 replacement method for signature 'ToxicoSet,data.frame'
sampleInfo(object) <- value

## S4 method for signature 'ToxicoSet'
sampleNames(object)

## S4 replacement method for signature 'ToxicoSet,character'
sampleNames(object) <- value

## S4 method for signature 'ToxicoSet'
curation(object)

## S4 replacement method for signature 'ToxicoSet,list'
curation(object) <- value

## S4 method for signature 'ToxicoSet'
datasetType(object)

## S4 replacement method for signature 'ToxicoSet,character'
datasetType(object) <- value

## S4 method for signature 'ToxicoSet'
molecularProfiles(object, mDataType, assay)

## S4 replacement method for signature 'ToxicoSet,character,character,matrix'
molecularProfiles(object, mDataType, assay) <- value

## S4 method for signature 'ToxicoSet'
featureInfo(object, mDataType)

## S4 replacement method for signature 'ToxicoSet,character,data.frame'
featureInfo(object, mDataType) <- value

## S4 method for signature 'ToxicoSet,character'
phenoInfo(object, mDataType)

## S4 replacement method for signature 'ToxicoSet,character,data.frame'
phenoInfo(object, mDataType) <- value

## S4 method for signature 'ToxicoSet,character'
fNames(object, mDataType)

## S4 replacement method for signature 'ToxicoSet,character,character'
fNames(object, mDataType) <- value

## S4 method for signature 'ToxicoSet'
mDataNames(object)

## S4 replacement method for signature 'ToxicoSet'
mDataNames(object) <- value

## S4 method for signature 'ToxicoSet'
molecularProfilesSlot(object)

## S4 replacement method for signature 'ToxicoSet,list_OR_MAE'
molecularProfilesSlot(object) <- value

## S4 method for signature 'ToxicoSet'
sensitivityInfo(object, dimension, ...)

## S4 replacement method for signature 'ToxicoSet,data.frame'
sensitivityInfo(object, dimension, ...) <- value

## S4 method for signature 'ToxicoSet'
sensitivityMeasures(object)

## S4 replacement method for signature 'ToxicoSet,character'
sensitivityMeasures(object) <- value

## S4 method for signature 'ToxicoSet'
sensitivityProfiles(object)

## S4 replacement method for signature 'ToxicoSet,data.frame'
sensitivityProfiles(object) <- value
## S4 method for signature 'ToxicoSet'
sensitivityRaw(object)
## S4 replacement method for signature 'ToxicoSet,array'
sensitivityRaw(object) <- value
## S4 method for signature 'ToxicoSet'
treatmentResponse(object)
## S4 replacement method for signature 'ToxicoSet,list_OR_LongTable'
treatmentResponse(object) <- value
## S4 method for signature 'ToxicoSet'
sensNumber(object)
## S4 replacement method for signature 'ToxicoSet,matrix'
sensNumber(object) <- value
## S4 method for signature 'ToxicoSet'
pertNumber(object)
## S4 replacement method for signature 'ToxicoSet,array'
pertNumber(object) <- value

Arguments

... See details.
value See details.
object A CoreSet object.
mDataType character(1) The name of a molecular datatype to access from the molecularProfiles of a CoreSet object.
assay character(1) A valid assay name in the SummarizedExperiment of @molecularProfiles of a CoreSet object for data type mDataType.
dimension See details.

Details

treatmentInfo: data.frame Metadata for all treatments in a ToxicoSet object. Arguments:
  • object: ToxicoSet An object to retrieve treatment metadata from.
treatmentInfo<-: ToxicoSet object with updated treatment metadata. object. Arguments:
  • object: ToxicoSet An object to set treatment metadata for.
  • value: data.frame A new table of treatment metadata for object.
treatmentNames: character Names for all treatments in a ToxicoSet object. Arguments:
• object: ToxicoSet An object to retrieve treatment names from.

**treatmentNames<-**: ToxicoSet Object with updates treatment names. object. Arguments:

• object: ToxicoSet An object to set treatment names from.
• value: character A character vector of updated treatment names.

@annotation:

annotation: A list of ToxicoSet annotations with items: 'name', the name of the object; 'dateCreated', date the object was created; 'sessionInfo', the sessionInfo() when the object was created; 'call', the R constructor call; and 'version', the object version.

**annotation<-**: Setter method for the annotation slot. Arguments:

• value: a list of annotations to update the ToxicoSet with.

@dateCreated:

dateCreated: character(1) The date the ToxicoSet object was created, as returned by the date() function.

dateCreated<-: Update the 'dateCreated' item in the annotation slot of a ToxicoSet object. Arguments:

• value: A character(1) vector, as returned by the date() function.

name: character(1) The name of the ToxicoSet, retrieved from the @annotation slot.

name<-: Update the @annotation$name value in a ToxicoSet object.

• value: character(1) The name of the ToxicoSet object.

cellInfo: data.frame Metadata for all sample in a ToxicoSet object.

**sampleInfo<-**: assign updated sample annotations to the ToxicoSet object. Arguments:

• value: a data.frame object.

sampleNames: character Retrieve the rownames of the data.frame in the sample slot from a ToxicoSet object.

**sampleNames<-**: assign new rownames to the sampleInfo data.frame for a ToxicoSet object. Arguments:

• value: character vector of rownames for the sampleInfo(object) data.frame.

@curation:

curation: A list of curated mappings between identifiers in the ToxicoSet object and the original data publication. Contains three data.frames, 'cell' with cell-line ids and 'tissue' with tissue ids and 'drug' with drug ids.

curation<-: Update the curation slot of a ToxicoSet object. Arguments:

• value: A list of data.frames, one for each type of curated identifier. For a ToxicoSet object the slot should contain tissue, cell-line and drug id data.frames.
**datasetType slot:**

**datasetType**: character(1) The type treatment response in the sensitivity slot. Valid values are 'sensitivity', 'perturbation' or 'both'.

**datasetType**<:- Update the datasetType slot of a ToxicoSet object. Arguments:

- value: A character(1) vector with one of 'sensitivity', 'perturbation' or 'both'

**@molecularProfiles:**

**molecularProfiles**: matrix() Retrieve an assay in a SummarizedExperiment from the molecularProfiles slot of a ToxicoSet object with the specified mDataType. Valid mDataType arguments can be found with mDataNames(object). Exclude mDataType and assay to access the entire slot. Arguments:

- assay: Optional character(1) vector specifying an assay in the SummarizedExperiment of the molecularProfiles slot of the ToxicoSet object for the specified mDataType. If excluded, defaults to modifying the first assay in the SummarizedExperiment for the given mDataType.

**molecularProfiles**<:- Update an assay in a SummarizedExperiment from the molecularProfiles slot of a ToxicoSet object with the specified mDataType. Valid mDataType arguments can be found with mDataNames(object). Omit mDataType and assay to update the slot.

- assay: Optional character(1) vector specifying an assay in the SummarizedExperiment of the molecularProfiles slot of the ToxicoSet object for the specified mDataType. If excluded, defaults to modifying the first assay in the SummarizedExperiment for the given mDataType.
- value: A matrix of values to assign to the assay slot of the SummarizedExperiment for the selected mDataType. The rownames and column names must match the associated SummarizedExperiment.

**featureInfo**: Retrieve a DataFrame of feature metadata for the specified mDataType from the molecularProfiles slot of a ToxicoSet object. More specifically, retrieve the @rowData slot from the SummarizedExperiment from the @molecularProfiles of a ToxicoSet object with the name mDataType.

**featureInfo**<:- Update the featureInfo(object, mDataType) DataFrame with new feature metadata. Arguments:

- value: A data.frame or DataFrame with updated feature metadata for the specified molecular profile in the molecularProfiles slot of a ToxicoSet object.

**phenoInfo**: Return the @colData slot from the SummarizedExperiment of mDataType, containing sample-level metadata, from a ToxicoSet object.

**phenoInfo**<:- Update the @colData slot of the SummarizedExperiment of mDataType in the @molecularProfiles slot of a ToxicoSet object. This updates the sample-level metadata in-place.

- value: A data.frame or DataFrame object where rows are samples and columns are sample metadata.

**fNames**: character() The features names from the rowData slot of a SummarizedExperiment of mDataType within a ToxicoSet object.

**fNames**: Updates the rownames of the feature metadata (i.e., rowData) for a SummarizedExperiment of mDataType within a ToxicoSet object.
• value: character() A character vector of new features names for the rowData of the SummarizedExperiment of mDataType in the @molecularProfiles slot of a ToxicoSet object. Must be the same length as nrow(featureInfo(object, mDataType)), the number of rows in the feature metadata.

mDataNames: character Retrieve the names of the molecular data types available in the molecularProfiles slot of a ToxicoSet object. These are the options which can be used in the mDataType parameter of various molecularProfiles slot accessor methods.

mDataNames: Update the molecular data type names of the molecularProfiles slot of a ToxicoSet object. Arguments:

• value: character vector of molecular datatype names, with length equal to length(molecularProfilesSlot(object))

molecularProfilesSlot: Return the contents of the @molecularProfiles slot of a ToxicoSet object. This will either be a list or MultiAssayExperiment of SummarizedExperiments.

molecularProfilesSlot<-: Update the contents of the @molecularProfiles slot of a ToxicoSet object. Arguments:

• value: A list or MultiAssayExperiment of SummarizedExperiments. The list and assays should be named for the molecular datatype in each SummarizedExperiment.

@treatmentResponse:

Arguments:

• dimension: Optional character(1) One of 'treatment', 'sample' or 'assay' to retrieve rowData, colData or the 'assay_metadata' assay from the ToxicoSet @sensitivity LongTable object, respectively. Ignored with warning if @treatmentResponse is not a LongTable object.

• ...: Additional arguments to the rowData or colData. LongTable methods. Only used if the sensitivity slot contains a LongTable object instead of a list and the dimension argument is specified.

Methods:

sensitivityInfo: DataFrame or data.frame of sensitivity treatment combo by sample metadata for the ToxicoSet object. When the dimension parameter is used, it allows retrieval of the dimension specific metadata from the LongTable object in @treatmentResponse of a ToxicoSet object.

sensitivityInfo<-: Update the @treatmentResponse slot metadata for a ToxicoSet object. When used without the dimension argument is behaves similar to the old ToxicoSet implementation, where the @treatmentResponse slot contained a list with a $info data.frame item. When the dimension argument is used, more complicated assignments can occur where 'sample' modifies the @sensitivity LongTable colData, 'treatment' the rowData and 'assay' the 'assay_metadata' assay. Arguments:

• value: A data.frame of treatment response experiment metadata, documenting experiment level metadata (mapping to treatments and samples). If the @treatmentResponse slot doesn’t contain a LongTable and dimension is not specified, you can only modify existing columns as returned by sensitivityInfo(object).
sensitivityMeasures: Get the 'sensitivityMeasures' available in a ToxicoSet object. Each measure represents some summary of sample sensitivity to a given treatment, such as ic50, ec50, AUC, AAC, etc. The results are returned as a character vector with all available metrics for the PSet object.

sensitivityMeasures: Update the sensitivity measure in a ToxicoSet object. These values are the column names of the 'profiles' assay and represent various computed sensitivity metrics such as ic50, ec50, AUC, AAC, etc.

- value: A character vector of new sensitivity measure names, the then length of the character vector must match the number of columns of the 'profiles' assay, excluding metadata and key columns.

sensitivityProfiles: Return the sensitivity profile summaries from the sensitivity slot. This data.frame contains various sensitivity summary metrics, such as ic50, amax, EC50, aac, HS, etc as columns, with rows as treatment by sample experiments.

sensitivityProfiles<-: Update the sensitivity profile summaries the sensitivity slot. Arguments:
- value: A data.frame the same number of rows as as returned by sensitivityProfiles(object), but potentially modified columns, such as the computation of additional summary metrics.

sensitivityRaw: Access the raw sensitivity measurements for a ToxicoSet object. A 3D array where rows are experiment_ids, columns are doses and the third dimension is metric, either 'Dose' for the doses used or 'Viability' for the sample viability at that dose.

sensitivityRaw<-: Update the raw dose and viability data in a ToxicoSet.

- value: A 3D array object where rows are experiment_ids, columns are replicates and pages are c('Dose', 'Viability'), with the corresponding dose or viability measurement for that experiment_id and replicate.

dataNumber: Return a count of viability observations in a ToxicoSet object for each treatment-combo by sample combination.

dataNumber<-: Update the 'n' item, which holds a matrix with a count of treatment by sample-line experiment counts, in the list in @treatmentResponse slot of a ToxicoSet object. Will error when @sensitivity contains a LongTable object, since the counts are computed on the fly. Arguments:

- value: A matrix where rows are samples and columns are treatments, with a count of the number of experiments for each combination as the values.

dataNumber: array Summary of available perturbation experiments from in a ToxicoSet object. Returns a 3D array with the number of perturbation experiments per treatment and sample, and data type.

dataNumber<-: Update the @perturbation$n value in a ToxicoSet object, which stores a summary of the available perturbation experiments. Arguments:

- value: A new 3D array with the number of perturbation experiments per treatment and sample, and data type.

Value

Accessors: See details.

Setters: An updated CoreSet object, returned invisibly.
Examples

data(TGGATESsmall)
treatmentInfo(TGGATESsmall)

treatmentInfo(TGGATESsmall) <- treatmentInfo(TGGATESsmall)
treatmentNames(TGGATESsmall)
treatmentNames(TGGATESsmall) <- treatmentNames(TGGATESsmall)

## @annotation
annotation(TGGATESsmall)
annotation(TGGATESsmall) <- annotation(TGGATESsmall)
dateCreated(TGGATESsmall)

## dateCreated
dateCreated(TGGATESsmall) <- date()

name(TGGATESsmall)
name(TGGATESsmall) <- 'new_name'
sampleInfo(TGGATESsmall) <- sampleInfo(TGGATESsmall)
sampleNames(TGGATESsmall)
sampleNames(TGGATESsmall) <- sampleNames(TGGATESsmall)

## curation
curation(TGGATESsmall)
curation(TGGATESsmall) <- curation(TGGATESsmall)
datasetType(TGGATESsmall)
datasetType(TGGATESsmall) <- 'both'

# No assay specified
molecularProfiles(TGGATESsmall, 'rna') <- molecularProfiles(TGGATESsmall, 'rna')

# Specific assay
molecularProfiles(TGGATESsmall, 'rna', 'exprs') <-
molecularProfiles(TGGATESsmall, 'rna', 'exprs')

# Replace the whole slot
molecularProfiles(TGGATESsmall) <- molecularProfiles(TGGATESsmall)

featureInfo(TGGATESsmall, 'rna')
ToxicoSet-class

Class to contain Toxico-genomic Data
ToxicoSig

Description

The ToxicoSet (tSet) class was developed to contain and organise large ToxicGenomic datasets as well as provide useful tools for interacting with this data. Functions are included for exploring the relationship between survival fraction and gene expression in cultured human and rat tissues during exposure to a wide range of compounds. Features include plotting dose and exposure time curves, calculating AUC, fitting linear models and computing sensitivity signatures.

Value

An object of the ToxicoSet class

Slots

 annotation A list of annotation data about the ToxicoSet, including the $name and the session information for how the object was created, detailing the exact versions of R and all the packages used

molecularProfiles A list containing SummarizedExperiment type object for holding data for RNA, DNA, SNP and CNV measurements, with associated fData and pData containing the row and column metadata

sample A data.frame containing the annotations for all the cell lines profiled in the data set, across all data types

treatment A data.frame containing the annotations for all the drugs profiled in the data set, across all data types

treatmentResponse A list containing all the data for the sensitivity experiments, including $info, a data.frame containing the experimental info,$raw a 3D array containing raw data, $profiles, a data.frame containing sensitivity profiles statistics, and $n, a data.frame detailing the number of experiments for each cell-drug pair

perturbation A list containing $n, a data.frame summarizing the available perturbation data,
curation A list containing mappings for $treatment, sample, tissue names used in the data set to universal identifiers used between different ToxicoSet objects

datasetType A character string of 'sensitivity', 'perturbation', or both detailing what type of data can be found in the ToxicoSet, for proper processing of the data

ToxicoSig Constructor

Description

A user-friendly constructor to create ToxicoSig class objects. This function is implemented as an internal and should only be called for development purposes.
Usage

ToxicoSig(
  Data = array(NA, dim = c(0, 0, 0)),
  tSetName = "",
  DateCreated = date(),
  SigType = "sensitivity",
  SessionInfo = sessionInfo(),
  Call = "No Call Recorded",
  Arguments = list()
)

Arguments

Data
  'array' An array containing the data for constructing the ToxicoSig object

tSetName
  character(1) The name of the tSet used in the constructor

DateCreated
  date The data at time of running the constructor

SigType
  character A string of the experiment type

SessionInfo
  sessionInfo The current session info

Call
  character(1) A string

Arguments
  list A list of arguments passed to the constructor

Value

object A new ToxicoSig object

Description

Update the ToxicoSet class after changes in structure or API

Usage

## S4 method for signature 'ToxicoSet'
updateObject(object)

Arguments

object A ToxicoSet object to update the class structure for.

Value

ToxicoSet with update class structure.
Description

Usage

## S4 method for signature 'ToxicoSet,ANY,ANY,ANY'
x[i, j, ..., drop = FALSE]

Arguments

x tSet
i Cell lines to keep in tSet
j Drugs to keep in tSet
... further arguments
drop A boolean flag of whether to drop single dimensions or not

Value

Returns the subsetted tSet

Examples

tSet <- TGGATESsmall[sampleNames(TGGATESsmall), treatmentNames(TGGATESsmall)[seq_len(3)]]
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