Package 'ToxicoGx'

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Description Contains a set of functions to perform large-scale analysis of toxicogenomic data, providing a standardized data structure to hold information relevant to annotation, visualization and statistical analysis of toxicogenomic data.

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`availableTSets` *Return a table of ToxicoSets available for download*

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 *A 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

```
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

```
checkTSetStructure(TGGATESsmall)
```

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-Viablility) 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.

Usage

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

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

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 precentile 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 *Generic method for performing differential expression analysis on an S4 object using the limma package*

Description

Generic method for performing differential expression analysis on an S4 object using the limma package

Usage

```
computeLimmaDiffExpr(object, ...)
```

Arguments

`object`
: `S4` An S4 object to conduct differential expression analysis on.

`...`
: Allow new parameters to be added to this generic.

Value

To be defined by the method implementation.

computeLimmaDiffExpr,ToxicoSet-method

Conduct differential expression analysis using the limma R pacakge

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 with 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

```
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)
```

Arguments

x	ToxicoSet

Value

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

Examples

```
data(TGGATESsmall)
dim(TGGATESsmall)
```

---

downloadTSet *Download a ToxicoSet object*

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

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

Arguments

name	`Character` string, the name of the PhamracoSet 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

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

`drugGeneResponseCurve` *Compares gene expression for a specificed 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 ggplot plot + function() syntax.

Usage

```
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.

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

```
if (interactive()) {
  drugGeneResponseCurve(TGGATESsmall, dose = c("Control", "Low", "Middle"),
  mDataTypes="rna", drug = treatmentNames(TGGATESsmall)[1],
  duration = c("2", "8", "24"), features = "ENSG00000002726_at")
}
```

---

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

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

```
  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 inlcude 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 diagnostive 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

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

`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

```
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 witch 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 drugs 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 (estimateof 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 cotaining the gene names associated with the HCC geneset signature

Usage

```
data(HCC_sig)
```

Format

character

logLogisticRegression — *Fits curves of the form E = E_inf + (1 - E_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

```
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

Value

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

Examples

```
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 funtion 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

```
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 prefered 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 subsetted
`cell_lines`	A list or vector of cell names as used in the dataset to which the object will be subsetted. 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 subsetted. 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 subsetted. 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

Examples

```
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 SummarizedExperiment object, with one Assay corresponding to a requested drug.

Usage

```
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

summary.stat	character which summary method to use if there are repeated cell_lines? Choices are "mean", "median", "first", or "last"
fill.missing	boolean should the missing cell lines not in the molecular data object be filled in with missing values?
summarize	A flag which when set to FALSE (defaults to TRUE) disables summarizing and returns the data unchanged as a ExpressionSet
verbose	boolean should messages be printed

Value

SummarizedExperiment A SummarizedExperiment object with the molecular data summarized per cell line.

Examples

```
data(TGGATESsmall)
summMP <- ToxicoGx::summarizeMolecularProfiles(
  tSet = TGGATESsmall, mDataType = "rna",
  cell_lines=sampleNames(TGGATESsmall), drugs = head(treatmentNames(TGGATESsmall)),
  features = fNames(TGGATESsmall,"rna")[seq_len(100)], duration = "8",
  dose = c("Control", "High"), summary.stat = "median",
  fill.missing = TRUE, verbose=TRUE
  )

#subset into expression matrix for a requested drug
assays <- SummarizedExperiment::assays(summMP)[[treatmentNames(TGGATESsmall)[1]]]
#summarization of phenoData for requested experiments
phenoData <- SummarizedExperiment::colData(summMP)
#summarization of phenoData for requested experiments
featureData <- SummarizedExperiment::rowData(summMP) #featureData for requested experiments
```

---

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 senstitivity data of a ToxicoSet into drug-cell line pairs for a specified experiment duration.

Usage

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

```
  drugs = NULL,
  sensitivity.measure = "auc_recomputed",
  summary.stat = c("mean", "median", "first", "last", "max", "min"),
  fill.missing = TRUE,
  verbose = TRUE
)
```

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')
```

`TGGATESsmall` *TGGATESsmall dataset*

Description

Documentation for this dataset will be added at a later date. For now I just need this package to pass the CRAN checks! This dataset powers the example usage in the roxygen2 documentation for ToxicoGx.

Usage

```
data(TGGATESsmall)
```

Format

ToxicoSet object

References

Lamb et al. The Connectivity Map: using gene-expression signatures to connect small molecules, genes, and disease. Science, 2006.

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.

`sample` A `data.frame` containing the annotations for all the sample profiled in the data set, 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 indenifiers for each treatment, matching the `treatment` object.

`sensitivityRaw` A 3 Dimensional `array` contaning 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', 'preturbation', 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` *Accessing and modifying information in a* `CoreSet`

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`, retreived 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. Arugments:

- 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 accessors 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. Arguemnts:

- 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` `@sensitvity` `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` arugment is used, more complicated assignments can occur where 'sample' modifies the `@sensitvity` `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)`.

sensitivityMeaures: Get the 'sensitivityMeasures' available in a `ToxicoSet` object. Each measure reprents 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.

sensitivityMeaures: Update the sensitivity meaure in a `ToxicoSet` object. Thesee values are the column names of the 'profiles' assay and represent various compued sensitviity 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 matcht he 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 cotanins vaarious 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 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 sensitiity measurents 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.

sensitvityRaw<-: 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.

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

sensNumber<-: 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 `@sensitviity` 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.

pertNumber: `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.

pertNumber<-: 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')
```

```
featureInfo(TGGATESsmall, 'rna') <- featureInfo(TGGATESsmall, 'rna')

phenoInfo(TGGATESsmall, 'rna')

phenoInfo(TGGATESsmall, 'rna') <- phenoInfo(TGGATESsmall, 'rna')

fNames(TGGATESsmall, 'rna')

fNames(TGGATESsmall, 'rna') <- fNames(TGGATESsmall, 'rna')

mDataNames(TGGATESsmall)

mDataNames(TGGATESsmall) <- mDataNames(TGGATESsmall)

molecularProfilesSlot(TGGATESsmall)

molecularProfilesSlot(TGGATESsmall) <- molecularProfilesSlot(TGGATESsmall)

sensitivityInfo(TGGATESsmall)

sensitivityInfo(TGGATESsmall) <- sensitivityInfo(TGGATESsmall)

sensitivityMeasures(TGGATESsmall) <- sensitivityMeasures(TGGATESsmall)

sensitivityMeasures(TGGATESsmall) <- sensitivityMeasures(TGGATESsmall)

sensitivityProfiles(TGGATESsmall)

sensitivityProfiles(TGGATESsmall) <- sensitivityProfiles(TGGATESsmall)

head(sensitivityRaw(TGGATESsmall))

sensitivityRaw(TGGATESsmall) <- sensitivityRaw(TGGATESsmall)

treatmentResponse(TGGATESsmall)

treatmentResponse(TGGATESsmall) <- treatmentResponse(TGGATESsmall)

sensNumber(TGGATESsmall)

sensNumber(TGGATESsmall) <- sensNumber(TGGATESsmall)

pertNumber(TGGATESsmall)

pertNumber(TGGATESsmall) <- pertNumber(TGGATESsmall)
```

`ToxicoSet-class` *Class to contain Toxico-genomic Data*

Description

The ToxicoSet (tSet) class was development 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 ranges 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 creating, 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` containg 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` containting `$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` *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 contiaining 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

`updateObject,ToxicoSet-method` *Update the ToxicoSet class after changes in it struture or API*

Description

Update the ToxicoSet class after changes in it struture 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.

[,ToxicoSet,ANY,ANY,ANY-method
[

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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