# Package: CoreGx (via r-universe)

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Type Package

**Title** Classes and Functions to Serve as the Basis for Other 'Gx' Packages

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**Description** A collection of functions and classes which serve as the foundation for our lab's suite of R packages, such as 'PharmacoGx' and 'RadioGx'. This package was created to abstract shared functionality from other lab package releases to increase ease of maintainability and reduce code repetition in current and future 'Gx' suite programs. Major features include a 'CoreSet' class, from which 'RadioSet' and 'PharmacoSet' are derived, along with get and set methods for each respective slot. Additional functions related to fitting and plotting dose response curves, quantifying statistical correlation and calculating area under the curve (AUC) or survival fraction (SF) are included. For more details please see the included documentation, as well as: Smirnov, P., Safikhani, Z., El-Hachem, N., Wang, D., She, A., Olsen, C., Freeman, M., Selby, H., Gendoo, D., Grossman, P., Beck, A., Aerts, H., Lupien, M., Goldenberg, A. (2015) <doi:10.1093/bioinformatics/btv723>. Manem, V., Labie, M., Smirnov, P., Kofia, V., Freeman, M., Koritzinksy, M., Abazeed, M., Haibe-Kains, B., Bratman, S. (2018) <doi:10.1101/449793>.

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Convenience function for converting R code to a call

## Description

This is used to pass through unevaluated R expressions into subset and [, where they will be evaluated in the correct context.

## Usage

.(...)

## **Arguments**

... pairlist One or more R expressions to convert to calls.

#### Value

call An R call object containing the quoted expression.

## **Examples**

```
.(sample_line1 == 'A2058')
```

.assayToBumpyMatrix

Convert a LongTable assay into a BumpyMatrix object

## Description

Convert a LongTable assay into a BumpyMatrix object

## Usage

```
.assayToBumpyMatrix(LT, assay, rows, cols, sparse = TRUE)
```

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## **Arguments**

LT	LongTable with assay to convert into BumpyMatrix
assay	$\label{eq:character} \mbox{character(1) A valid assay name in LT, as returned by $\mbox{assayNames(LT)}$.}$
rows	character() The rownames associated with the assay rowKey
cols	character() The names associated with the assay colKey
sparse	logical(1) Should the BumpyMatrix be sparse (i.e., is the assay sparse).

## Value

BumpyMatrix containing the data from assay.

.fitCurve2 Curve fitting via stats::optim L-BFGS-B with fall-back grid/pattern search if convergence is not achieved.

## **Description**

Function to fit curve via stats::optim

## Usage

```
.fitCurve2(
 par,
 х,
  у,
  fn,
  loss,
  lower = -Inf,
  upper = Inf,
  precision = 1e-04,
 density = c(2, 10, 5),
  step = 0.5/density,
  loss_args = list(),
  span = 1,
 optim_only = FALSE,
 control = list(factr = 1e-08, ndeps = rep(1e-04, times = length(par)), trace = 0)
)
```

#### **Arguments**

.fitCurve2

У	numeric Target output values to optimze fn against.
fn	function A function to optimize. Any fn arguments passed via will be treated as constant and removed from the optimization. It is assumed that the first argument is the x value to optimize over and any subsequent arguments are free parameters to be optimized. Transformed to be optim compatible via make_optim_function is the first argument isn't already par.
loss	character(1) or function Either the name of one of the bundled loss functions (see details) or a custom loss function to compute for the output of $fn$ over $x$ .
lower	numeric(1) Lower bound for parameters. Parallel to par.
upper	numeric(1) Upper bound for paramteres. Parallel to par.
precision	numeric smallest step size used in pattern search, once step size drops below this value, the search terminates.
density	numeric how many points in the dimension of each parameter should be evaluated (density of the grid)
step	initial step size for pattern search.
	pairlist Fall through arguments to fn.
loss_args	list Additional argument to the loss function. These get passed to losss via do.call analagously to using $\dots$
span	numeric Can be safely kept at 1, multiplicative ratio for initial step size in pattern search. Must be larger than precision.
optim_only	logical(1) Should the fall back methods when optim fails be skipped? Default is FALSE.
control	list List of control parameters to pass to optim. See ?optim for details.

## **Details**

TODO

## Value

numeric Vector of optimal parameters for fn fit against y on the values of x.

## Examples

```
nresponse <- response + rnorm(length(response), sd=sd(response)*0.1) # add noise</pre>
 # 3-parameter optimization
 3par <- .fitCurve2(</pre>
      par=c(Emax, EC50, lambda),
      x=doses,
      y=nresponse,
      fn=hillEqn,
      Emin=Emin, # set this as constant in the function being optimized (via ...)
      loss=.normal_loss,
      loss_args=list(trunc=FALSE, n=1, scale=0.07),
      upper=c(1, max(doses), 6),
      lower=c(0, min(doses), 0)
 # 2-parameter optimization
 2par <- .fitCurve2(</pre>
      par=c(Emax, EC50),
      x=doses,
      y=nresponse,
      fn=hillEqn,
      Emin=Emin, # set this as constant in the function being optimized (via ...)
      lambda=1,
      loss=.normal_loss,
      loss_args=list(trunc=FALSE, n=1, scale=0.07),
      upper=c(1, max(doses)),
      lower=c(0, min(doses))
 )
## End(Not run)
```

.longTableToSummarizedExperiment

Convert LongTable to gDR Style SummarizedExperiment

## Description

Convert LongTable to gDR Style SummarizedExperiment

#### Usage

```
.longTableToSummarizedExperiment(LT, assay_names)
```

#### **Arguments**

```
LT LongTable to convert to gDR SummarizedExperiment format.

assay_names character() Names to rename the assays to. These are assumed to be in the same order as assayNames(LT).
```

#### Value

SummarizedExperiment object with all assay from LT as BumpyMatrixes.

```
aggregate, data.table-method
```

Functional S4 API for aggregation over a data.table object.

## Description

Compute a group-by operation over a data. table in a functional, pipe compatible format.

#### Usage

```
## S4 method for signature 'data.table'
aggregate(
    x,
    by,
    ...,
    subset = TRUE,
    nthread = 1,
    progress = TRUE,
    BPPARAM = NULL,
    enlist = TRUE,
    moreArgs = list()
)
```

## **Arguments**

x data.table to compute aggregation ov
--

by character One or more valid column names in x to compute groups using.

.. call One or more aggregations to compute for each group by in x. If you name aggregation calls, that will be the column name of the value in the resulting data.table otherwise a default name will be parsed from the function name and its first argument, which is assumed to be the name of the column being

aggregated over.

subset call An R call to evaluate before perfoming an aggregate. This allows you to

aggregate over a subset of columns in an assay but have it be assigned to the parent object. Default is TRUE, which includes all rows. Passed through as the

 $i \ argument \ in \ [ \ . \ data. \ table.$ 

nthread numeric(1) Number of threads to use for split-apply-combine parallelization.

Uses BiocParllel::bplapply if nthread > 1 or you pass in BPPARAM. Does not modify data.table threads, so be sure to use setDTthreads for reasonable nested

parallelism. See details for performance considerations.

progress logical(1) Display a progress bar for parallelized computations? Only works

if bpprogressbar<- is defined for the current BiocParallel back-end.

BPPARAM BiocParallelParam object. Use to customized the the parallization back-end

of bplapply. Note, nthread over-rides any settings from BPPARAM as long as

bpworkers<- is defined for that class.

enlist logical(1) Default is TRUE. Set to FALSE to evaluate the first call in . . . within

data.table groups. See details for more information.

moreArgs list() A named list where each item is an argument one of the calls in ...

which is not a column in the table being aggregated. Use to further parameterize you calls. Please note that these are not added to your aggregate calls unless you

specify the names in the call.

#### **Details**

This S4 method override the default aggregate method for a data.frame and as such you need to call aggregate.data.frame directly to get the original S3 method for a data.table.

### **Use of Non-Standard Evaluation:**

Arguments in . . . are substituted and wrapped in a list, which is passed through to the j argument of [.data.table internally. The function currently tries to build informative column names for unnamed arguments in . . . by appending the name of each function call with the name of its first argument, which is assumed to be the column name being aggregated over. If an argument to . . . is named, that will be the column name of its value in the resulting data.table.

#### **Enlisting:**

The primary use case for enlist=FALSE is to allow computation of dependent aggregations, where the output from a previous aggregation is required in a subsequent one. For this case, wrap your call in { and assign intermediate results to variables, returning the final results as a list where each list item will become a column in the final table with the corresponding name. Name inference is disabled for this case, since it is assumed you will name the returned list items appropriately. A major advantage over multiple calls to aggregate is that the overhead of parallelization is paid only once even for complex multi-step computations like fitting a model, capturing its paramters, and making predictions using it. It also allows capturing arbitrarily complex calls which can be recomputed later using the update, TreatmentResponseExperiment-method A potential disadvantage is increased RAM usage per thread due to storing intermediate values in variables, as well as any memory allocation overhead associate therewith.

#### Value

data.table of aggregated results with an aggregations attribute capturing metadata about the last aggregation performed on the table.

aggregate, LongTable-method

Functional API for aggregation over a LongTable or inheriting class

#### **Description**

Compute a group-by operation over a LongTable object or it's inhering classes.

#### Usage

```
## S4 method for signature 'LongTable'
aggregate(
 х,
 assay,
 by,
  . . . ,
  subset = TRUE,
  nthread = 1,
  progress = TRUE,
 BPPARAM = NULL,
 enlist = TRUE,
 moreArgs = list()
)
```

## **Arguments**

X	LongTable or inheriting class to compute aggregation on.

character(1) The assay to aggregate over. assay

character One or more valid column names in x to compute groups using. by

> call One or more aggregations to compute for each group by in x. If you name aggregation calls, that will be the column name of the value in the resulting data.table otherwise a default name will be parsed from the function name and its first argument, which is assumed to be the name of the column being

aggregated over.

subset call An R call to evaluate before perforing an aggregate. This allows you to

aggregate over a subset of columns in an assay but have it be assigned to the parent object. Default is TRUE, which includes all rows. Passed through as the

i argument in [.data.table.

nthread numeric(1) Number of threads to use for split-apply-combine parallelization.

> Uses BiocParllel::bplapply if nthread > 1 or you pass in BPPARAM. Does not modify data.table threads, so be sure to use setDTthreads for reasonable nested

parallelism. See details for performance considerations.

logical(1) Display a progress bar for parallelized computations? Only works progress

if bpprogressbar<- is defined for the current BiocParallel back-end.

**BPPARAM** BiocParallelParam object. Use to customized the the parallization back-end

of bplapply. Note, nthread over-rides any settings from BPPARAM as long as

bpworkers<- is defined for that class.

enlist logical(1) Default is TRUE. Set to FALSE to evaluate the first call in . . . within

data.table groups. See details for more information.

moreArgs list() A named list where each item is an argument one of the calls in ...

> which is not a column in the table being aggregated. Use to further parameterize you calls. Please note that these are not added to your aggregate calls unless you

specify the names in the call.

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#### **Details**

#### **Use of Non-Standard Evaluation:**

Arguments in . . . are substituted and wrapped in a list, which is passed through to the j argument of [.data.table internally. The function currently tries to build informative column names for unnamed arguments in . . . by appending the name of each function call with the name of its first argument, which is assumed to be the column name being aggregated over. If an argument to . . . is named, that will be the column name of its value in the resulting data.table.

#### **Enlisting:**

The primary use case for enlist=FALSE is to allow computation of dependent aggregations, where the output from a previous aggregation is required in a subsequent one. For this case, wrap your call in { and assign intermediate results to variables, returning the final results as a list where each list item will become a column in the final table with the corresponding name. Name inference is disabled for this case, since it is assumed you will name the returned list items appropriately. A major advantage over multiple calls to aggregate is that the overhead of parallelization is paid only once even for complex multi-step computations like fitting a model, capturing its paramters, and making predictions using it. It also allows capturing arbitrarily complex calls which can be recomputed later using the update, TreatmentResponseExperiment-method A potential disadvantage is increased RAM usage per thread due to storing intermediate values in variables, as well as any memory allocation overhead associate therewith.

#### Value

```
data. table of aggregation results.
```

## See Also

```
data.table::[.data.table,BiocParallel::bplapply
```

aggregate2

Functional API for data.table aggregation which allows capture of associated aggregate calls so they can be recomputed later.

## **Description**

Functional API for data.table aggregation which allows capture of associated aggregate calls so they can be recomputed later.

#### Usage

```
aggregate2(
   x,
   by,
   ...,
   nthread = 1,
   progress = interactive(),
   BPPARAM = NULL,
```

aggregate2

```
enlist = TRUE,
moreArgs = list()
)
```

#### **Arguments**

x data.table
--------------

by character One or more valid column names in x to compute groups using.

... call One or more aggregations to compute for each group by in x. If you name aggregation calls, that will be the column name of the value in the resulting data.table otherwise a default name will be parsed from the function name and its first argument, which is assumed to be the name of the column being

aggregated over.

nthread numeric(1) Number of threads to use for split-apply-combine parallelization.

Uses BiocParllel::bplapply if nthread > 1 or you pass in BPPARAM. Does not modify data.table threads, so be sure to use setDTthreads for reasonable nested

parallelism. See details for performance considerations.

progress logical(1) Display a progress bar for parallelized computations? Only works

if bpprogressbar<- is defined for the current BiocParallel back-end.

BPPARAM BiocParallelParam object. Use to customized the parallization back-end

of bplapply. Note, nthread over-rides any settings from BPPARAM as long as

bpworkers<- is defined for that class.

enlist logical(1) Default is TRUE. Set to FALSE to evaluate the first call in . . . within

data.table groups. See details for more information.

moreArgs list() A named list where each item is an argument one of the calls in ...

which is not a column in the table being aggregated. Use to further parameterize you calls. Please note that these are not added to your aggregate calls unless you

specify the names in the call.

#### **Details**

#### **Use of Non-Standard Evaluation:**

Arguments in . . . are substituted and wrapped in a list, which is passed through to the j argument of [.data.table internally. The function currently tries to build informative column names for unnamed arguments in . . . by appending the name of each function call with the name of its first argument, which is assumed to be the column name being aggregated over. If an argument to . . . is named, that will be the column name of its value in the resulting data.table.

#### **Enlisting:**

The primary use case for enlist=FALSE is to allow computation of dependent aggregations, where the output from a previous aggregation is required in a subsequent one. For this case, wrap your call in { and assign intermediate results to variables, returning the final results as a list where each list item will become a column in the final table with the corresponding name. Name inference is disabled for this case, since it is assumed you will name the returned list items appropriately. A major advantage over multiple calls to aggregate is that the overhead of parallelization is paid only once even for complex multi-step computations like fitting a model, capturing its paramters, and making predictions using it. It also allows capturing arbitrarily complex calls which can be

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recomputed later using the update, TreatmentResponseExperiment-method A potential disadvantage is increased RAM usage per thread due to storing intermediate values in variables, as well as any memory allocation overhead associate therewith.

#### Value

data.table of aggregation results.

#### See Also

```
data.table::[.data.table, BiocParallel::bplapply
```

amcc

Calculate an Adaptive Matthews Correlation Coefficient

## **Description**

This function calculates an Adaptive Matthews Correlation Coefficient (AMCC) for two vectors of values of the same length. It assumes the entries in the two vectors are paired. The Adaptive Matthews Correlation Coefficient for two vectors of values is defined as the Maximum Matthews Coefficient over all possible binary splits of the ranks of the two vectors. In this way, it calculates the best possible agreement of a binary classifier on the two vectors of data. If the AMCC is low, then it is impossible to find any binary classification of the two vectors with a high degree of concordance.

#### Usage

```
amcc(x, y, step.prct = 0, min.cat = 3, nperm = 1000, nthread = 1, ...)
```

#### **Arguments**

x, y	Two paired vectors of values. Could be replicates of observations for the same experiments for example.
step.prct	Instead of testing all possible splits of the data, it is possible to test steps of a percentage size of the total number of ranks in x/y. If this variable is 0, function defaults to testing all possible splits.
min.cat	The minimum number of members per category. Classifications with less members fitting into both categories will not be considered.
nperm	The number of perumatation to use for estimating significance. If 0, then no p-value is calculated.
nthread	Number of threads to parallize over. Both the AMCC calculation and the permutation testing is done in parallel.
	Additional arguments

## Value

Returns a list with two elements. \$amcc contains the highest 'mcc' value over all the splits, the p value, as well as the rank at which the split was done.

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#### **Examples**

```
x \leftarrow c(1,2,3,4,5,6,7)

y \leftarrow c(1,3,5,4,2,7,6)

amcc(x,y, min.cat=2)
```

as

 $Coerce \ a \ LongTable \ to \ a \ TreatmentResponseExperiment$ 

## **Description**

Coerce a LongTable into a data.table.

Currently only supports coercing to data.table or data.frame

Coerce a data.table with the proper configuration attributes back to a LongTable

## **Arguments**

from

A LongTableDataMapper to coerce.

#### Value

The data in object, as the child-class TreatmentResponseExperiment.

A data.table with the data from a LongTable.

data.table containing the data from the LongTable, with the 'longTableDataMapper' attribute containg the metadata needed to reverse the coercing operation.

LongTable object configured with the longTableDataMapper

data.table with long format of data in from

data. frame with long format of data in from.

SummarizedExperiment with each assay as a BumpyMatrix

A TREDataMapper object.

#### See Also

```
TreatmentResponseExperiment
BumpyMatrix::BumpyMatrix
```

## **Examples**

```
data(clevelandSmall_cSet)
TRE <- as(treatmentResponse(clevelandSmall_cSet),
    "TreatmentResponseExperiment")
TRE
as(merckLongTable, 'data.table')</pre>
```

as.long.table

```
dataTable <- as(merckLongTable, 'data.table')
print(attr(dataTable, 'longTableDataMapper')) # Method doesn't work without this
as(dataTable, 'LongTable')

SE <- molecularProfilesSlot(clevelandSmall_cSet)[[1]]
as(SE, 'data.table')

SE <- molecularProfilesSlot(clevelandSmall_cSet)[[1]]
as(SE, 'data.frame')</pre>
```

as.long.table

Coerce from data.table to LongTable

#### **Description**

Coerce a data.table with the proper configuration attributes back to a LongTable

#### Usage

```
as.long.table(x)
```

#### **Arguments**

Х

A data.frame with the 'longTableDataMapper' attribute, containing three lists named assayCols, rowDataCols and colDataCols. This attribute is automatically created when coercing from a LongTable to a data.table.

#### Value

LongTable object configured with the longTableDataMapper

## **Examples**

```
dataTable <- as(merckLongTable, 'data.table')
print(attr(dataTable, 'longTableDataMapper')) # Method doesn't work without this
as.long.table(dataTable)</pre>
```

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assayCols

Generic to access the assay columns of a rectangular object.

## Description

Generic to access the assay columns of a rectangular object.

## Usage

```
assayCols(object, ...)
```

## **Arguments**

object S4 An object to get assay ids from.
... Allow new arguments to this generic.

#### Value

Depends on the implemented method.

## **Examples**

```
print("Generics shouldn't need examples?")
```

assayIndex

Retrieve and assayIndex

## **Description**

Retrieve and assayIndex

## Usage

```
assayIndex(x, ...)
```

## **Arguments**

x An S4 object.

... pairlist Allow definition of new parameters for implementations of this generic.

#### Value

An object representing the "assayIndex" of an S4 object.

assignment-immutable

## **Examples**

```
print("Generics shouldn't need examples?")
```

assayKeys

Retrieve a set of assayKeys

## **Description**

Retrieve a set of assayKeys

#### Usage

```
assayKeys(x, ...)
```

## **Arguments**

x An S4 object.

... pairlist Allow definition of new parameters for implementations of this generic.

### Value

An object representing the "assayKeys" of an S4 object.

## **Examples**

```
print("Generics shouldn't need examples?")
```

## **Description**

Prevents modification of objects labelled with the "immutable" S3-class by intercepting assignment during S3-method dispatch and returning an error.

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## Usage

```
\method{subset}{immutable}(object, ...) <- value

## S3 replacement method for class 'immutable'
object[...] <- value

## S3 replacement method for class 'immutable'
object[[...]] <- value

## S3 replacement method for class 'immutable'
object$... <- value

## S3 replacement method for class 'immutable'
names(x) <- value

## S3 replacement method for class 'immutable'
names(x) <- value

## S3 replacement method for class 'immutable'
dimnames(x) <- value

\method{colnames}{immutable}(x) <- value

\method{rownames}{immutable}(x) <- value</pre>
```

#### **Arguments**

object, x An R object inherting from the "immutable" S3-class.
... Catch subset arguments for various dimensions.
value Not used.

#### Value

None, throws an error.

#### **Examples**

```
immutable_df <- immutable(data.frame(a=1:5, b=letters[1:5]))
# return immutable data.frame
immutable_df[1:4, ]
# return immutable vector
immutable_df$a</pre>
```

buildComboProfiles

Build an assay table with an S4 object.

## **Description**

Build an assay table with an S4 object.

### Usage

```
buildComboProfiles(object, ...)
```

## Arguments

object S4 An S4 object a list-like slot containing assays for the object.

... Allow new arguments to be defined for this generic.

#### Value

data.table.

## **Examples**

```
"This is a generic method!"
```

buildComboProfiles,LongTable-method

Build an assay table with selected assay profiles for drug combinations

## **Description**

Build an assay table with selected assay profiles for drug combinations

## Usage

```
## S4 method for signature 'LongTable'
buildComboProfiles(object, profiles)
```

#### **Arguments**

object LongTable or inheriting class containing curated drug combination data.

profiles character a vector of profile names, i.e., column names of assays.

## Value

A data.table containing fields treatment1id, treatment1dose, treatment2id, treatment2dose, sampleid, which are used as keys to keep track of profiles, along with columns of selected profiles from their assays. Each \*\_1 is the monothearpy profile of treatment 1 in the combination, and the same rule applies to treatment 2.

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### **Examples**

```
## Not run:
combo_profile_1 <- buildComboProfiles(tre, c("auc", "SCORE"))
combo_profile_2 <- buildComboProfiles(tre, c("HS", "EC50", "E_inf", "ZIP"))
## End(Not run)</pre>
```

buildLongTable

Build a LongTable object

## **Description**

Build a LongTable object

## Usage

```
buildLongTable(from, ...)
```

## **Arguments**

from What to build the LongTable from?

... pairlist Allow definition of new parameters for implementations of this generic.

#### Value

Depends on the implemented method

## **Examples**

```
print("Generics shouldn't need examples?")
```

buildLongTable, character-method

LongTable build method from character

## **Description**

LongTable Create a LongTable object from a single .csv file

#### Usage

```
## S4 method for signature 'character'
buildLongTable(from, rowDataCols, colDataCols, assayCols)
```

#### **Arguments**

from character Path to the .csv file containing the data and metadata from which to

build the LongTable.

rowDataCols list List with two character vectors, the first specifying one or more columns

to be used as cell identifiers (e.g., cell-line name columns) and the second con-

taining any additional metadata columns related to the cell identifiers.

colDataCols list List with two character vectors, the first specifying one or more columns

to be used as column identifiers (e.g., drug name columns) and the second containing any additional metadata columns related to the column identifiers.

assayCols list A named list of character vectors specifying how to parse assay columns

into a list of data.tables. Each list data.table will be named for the name of corresponding list item and contain the columns specified in the character vector

of column names in each list item.

#### Value

A LongTable object containing one or more assays, indexed by rowID and colID.

#### **Description**

Create a LongTable object from a single data.table or data.frame object.

#### Usage

```
## S4 method for signature 'data.frame'
buildLongTable(from, rowDataCols, colDataCols, assayCols)
```

## Arguments

from character Path to the .csv file containing the data and metadata from which to

build the LongTable.

rowDataCols list List with two character vectors, the first specifying one or more columns

to be used as cell identifiers (e.g., cell-line name columns) and the second containing any additional metadata columns related to the cell identifiers. If you wish to rename any of these columns, assign the new names to their respective

character vectors.

colDataCols list List with two character vectors, the first specifying one or more columns

to be used as column identifiers (e.g., drug name columns) and the second containing any additional metadata columns related to the column identifiers. If you wish to rename any of these columns, assign the new names to their respective

character vectors.

assayCols

list A named list of character vectors specifying how to parse assay columns into a list of data.tables. Each list data.table will be named for the name of corresponding list item and contain the columns specified in the character vector of column names in each list item. If there are no names for assayCols, the assays will be numbered by instead.

#### Value

A LongTable object containing one or more assays, indexed by rowID and colID.

```
buildLongTable,list-method
```

LongTable build method from list

## Description

Create a LongTable object from a list containing file paths, data.frames and data.tables.

#### Usage

```
## S4 method for signature 'list'
buildLongTable(from, rowDataCols, colDataCols, assayCols)
```

## **Arguments**

from	list A list containing any combination of character file paths, data.tables and data.frames which will be used to construct the LongTable.
rowDataCols	list List with two character vectors, the first specifying one or more columns to be used as cell identifiers (e.g., cell-line name columns) and the second containing any additional metadata columns related to the cell identifiers.
colDataCols	list List with two character vectors, the first specifying one or more columns to be used as column identifiers (e.g., drug name columns) and the second containing any additional metadata columns related to the column identifiers.
assayCols	list A named list of character vectors specifying how to parse assay columns into a list of data.tables. Each list data.table will be named for the name of corresponding list item and contain the columns specified in the character vector of column names in each list item.

#### Value

A LongTable object constructed with the data in from.

#### **Examples**

```
## Not run:
assayList <- assays(merckLongTable, withDimnames=TRUE)
rowDataCols <- list(rowIDs(merckLongTable), rowMeta(merckLongTable))
colDataCols <- list(colIDs(merckLongTable), colMeta(merckLongTable))
assayCols <- assayCols(merckLongTable)
longTable <- buildLongTable(from=assayList, rowDataCols, colDataCols, assayCols)
## End(Not run)</pre>
```

c.immutable

Intercept concatenation for "immutable" class objects to return another "immutable" class object.

## **Description**

Ensures that c and append to an "immutable" class object return an immutable class object.

#### Usage

```
## S3 method for class 'immutable' c(x, ...)
```

#### **Arguments**

x An R object inheriting from the "immutable" S3-clas

. . . Objects to concatenate to x.

#### Value

x with one or more values appended to it.

checkColumnCardinality

Search a data.frame for 1:cardinality relationships between a group of columns (your identifiers) and all other columns.

#### **Description**

Search a data.frame for 1:cardinality relationships between a group of columns (your identifiers) and all other columns.

#### Usage

```
checkColumnCardinality(df, group, cardinality = 1, ...)
```

checkCsetStructure 25

## **Arguments**

df	A data.frame to search for 1:cardinality mappings with the columns in group. $ \\$
group	A character vector of one or more column names to check the cardinality of other columns against.
cardinality	The cardinality of to search for (i.e., 1:cardinality) relationships with the combination of columns in group. Defaults to 1 (i.e., 1:1 mappings).
	Fall through arguments to data.table::[. For developer use. One use case is setting verbose=TRUE to diagnose slow data.table operations.

#### Value

A character vector with the names of the columns with cardinality of 1:cardinality with the columns listed in group.

### **Examples**

```
df <- rawdata(exampleDataMapper)
checkColumnCardinality(df, group='treatmentid')</pre>
```

checkCsetStructure A

A function to verify the structure of a CoreSet

## **Description**

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

## Usage

```
checkCsetStructure(object, plotDist = FALSE, result.dir = tempdir())
```

## Arguments

object A CoreSet to be verified

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 this R sessions tempdir().

#### Value

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

### **Examples**

checkCsetStructure(clevelandSmall\_cSet)

clevelandSmall\_cSet

Cleaveland\_mut RadioSet subsetted and cast as CoreSet

### **Description**

This dataset is just a dummy object derived from the Cleveland\_mut RadioSet in the RadioGx R package. It's contents should not be interpreted and it is only present to test the functions in this package and provide examples

### Usage

```
data(clevelandSmall_cSet)
```

#### **Format**

CoreSet object

#### References

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

 $\verb|colData,LongTableDataMapper-method|\\$ 

Convenience method to subset the colData out of the rawdata slot using the assigned colDataMap metadata.

## Description

Convenience method to subset the colData out of the rawdata slot using the assigned colDataMap metadata.

#### Usage

```
## S4 method for signature 'LongTableDataMapper'
colData(x, key = TRUE)
```

#### **Arguments**

key

x LongTableDataMapper object with valid data in the rawdata and colDataMap

slots

logical(1) Should the table be keyed according to the id\_columns of the

colDataMap slot? This will sort the table in memory. Default is TRUE.

#### Value

data.table The colData as specified in the colDataMap slot.

```
colData, TREDataMapper-method
```

Convenience method to subset the colData out of the rawdata slot using the assigned colDataMap metadata.

## **Description**

Convenience method to subset the colData out of the rawdata slot using the assigned colDataMap metadata.

## Usage

```
## S4 method for signature 'TREDataMapper'
colData(x, key = TRUE)
```

## **Arguments**

x TREDataMapper object with valid data in the rawdata and colDataMap slots.

key logical(1) Should the table be keyed according to the id\_columns of the

colDataMap slot? This will sort the table in memory. Default is TRUE.

## Value

data.table The colData as specified in the colDataMap slot.

colIDs

Generic to access the row identifiers for an object.

## Description

Generic to access the row identifiers for an object.

## Usage

```
colIDs(object, ...)
```

## **Arguments**

object S4 An object to get column id columns from.

... ALlow new arguments to this generic

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## Value

Depends on the implemented method.

## **Examples**

```
print("Generics shouldn't need examples?")
```

collect\_fn\_params

Collects all function arguments other than the first into a single list parameter.

## Description

Useful for converting a regular function into a function amenable to optimization via stats::optim, which requires all free parameters be passed as a single vector par.

#### Usage

```
collect_fn_params(fn)
```

#### **Arguments**

fn

function A non-primitive function to refactor such that the first argument becomes the second argument and all other parameters must be passed as a vector to the first argument of the new function via the par parameter.

#### **Details**

Takes a function of the form f(x, ...), where ... is any number of additional function parameters (bot not literal ...!) and parses it to a function of the form f(par, x) where par is a vector of values for ... in the same order as the arguments appear in fn.

## Value

function A new non-primitive function where the first argument is par, which takes a vector of parameters being optimized, and the second argument is the old first argument to fn (usually x since this is the independent variable to optimize the function over).

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colMeta

Generic to access the column identifiers for a rectangular object.

#### **Description**

Generic to access the column identifiers for a rectangular object.

## Usage

```
colMeta(object, ...)
```

## Arguments

```
object S4 An object to get column metadata columns from.
... ALlow new arguments to this generic
```

#### Value

Depends on impemented method.

## **Examples**

```
print("Generics shouldn't need examples?")
```

connectivityScore

Function computing connectivity scores between two signatures

## Description

A function for finding the connectivity between two signatures, using either the GSEA method based on the KS statistic, or the gwc method based on a weighted spearman statistic. The GSEA analysis is implemented in the piano package.

## Usage

```
connectivityScore(
    x,
    y,
    method = c("fgsea", "gwc"),
    nperm = 10000,
    nthread = 1,
    gwc.method = c("spearman", "pearson"),
    ...
)
```

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## **Arguments**

X	A matrix with the first gene signature. In the case of GSEA the vector of values per gene for GSEA in which we are looking for an enrichment. In the case of gwc, this should be a matrix, with the per gene responses in the first column, and the significance values in the second.
у	A matrix with the second signature. In the case of GSEA, this is the vector of up and down regulated genes we are looking for in our signature, with the direction being determined from the sign. In the case of gwc, this should be a matrix of identical size to x, once again with the per gene responses in the first column, and their significance in the second.
method	character string identifying which method to use, out of 'fgsea' and 'gwc'
nperm	numeric, how many permutations should be done to determine significance through permutation testing? The minimum is 100, default is 1e4.
nthread	numeric, how many cores to run parallel processing on.
gwc.method	character, should gwc use a weighted spearman or pearson statistic?
	Additional arguments passed down to gsea and gwc functions

#### Value

numeric a numeric vector with the score and the p-value associated with it

#### References

F. Pozzi, T. Di Matteo, T. Aste, 'Exponential smoothing weighted correlations', The European Physical Journal B, Vol. 85, No 6, 2012. DOI: 10.1140/epjb/e2012-20697-x

Varemo, L., Nielsen, J. and Nookaew, I. (2013) Enriching the gene set analysis of genome-wide data by incorporating directionality of gene expression and combining statistical hypotheses and methods. Nucleic Acids Research. 41 (8), 4378-4391. doi: 10.1093/nar/gkt111

#### **Examples**

CoreGx-deprecated 31

CoreGx-deprecated

List of deprecated or defunct methods in the CoreGx R package.

#### **Description**

List of deprecated or defunct methods in the CoreGx R package.

#### **Details**

#### deprecated:

CoreSet: The CoreSet constructor is being updated to have a new API. This API is currently available via the CoreSet2 constructor. In Bioconductor 3.16, the old constructor will be renamed CoreSet2 and the new constructor will be renamed CoreSet.

#### defunct:

buildLongTable: This function no longer works as building a LongTable or TreatmentResponseExperiment now uses a DataMapper and the metaConstruct method. See vignette("LongTable") for a detailed description of how to create a LongTable object.

CoreSet

CoreSet constructor

#### **Description**

A constructor that simplifies the process of creating CoreSets, 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 CoreSet methods.

#### Usage

```
CoreSet(
  name,
 molecularProfiles = list(),
  sample = 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)),
  curationSample = data.frame(),
  curationTissue = data.frame(),
  curationTreatment = data.frame(),
  treatment = data.frame(),
  datasetType = c("sensitivity", "perturbation", "both"),
  verify = TRUE,
)
```

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#### **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.

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 containing the raw drug dose response data for the sen-

sitivity 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

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.

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?

... Catch and parse any renamed constructor arguments.

#### Details

#### WARNING::

Parameters to this function have been renamed!

- · cell is now sample
- drug is now treatment

## Value

An object of class CoreSet

## **Examples**

data(clevelandSmall\_cSet)
clevelandSmall\_cSet

CoreSet-accessors 33

CoreSet-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

```
## S4 method for signature 'CoreSet'
annotation(object)
## S4 replacement method for signature 'CoreSet,list'
annotation(object) <- value</pre>
## S4 method for signature 'CoreSet'
dateCreated(object)
## S4 replacement method for signature 'CoreSet, character'
dateCreated(object) <- value</pre>
## S4 method for signature 'CoreSet'
name(object)
## S4 replacement method for signature 'CoreSet'
name(object) <- value</pre>
## S4 method for signature 'CoreSet'
sampleInfo(object)
## S4 replacement method for signature 'CoreSet, data.frame'
sampleInfo(object) <- value</pre>
## S4 method for signature 'CoreSet'
sampleNames(object)
## S4 replacement method for signature 'CoreSet, character'
sampleNames(object) <- value</pre>
## S4 method for signature 'CoreSet'
treatmentInfo(object)
## S4 replacement method for signature 'CoreSet, data.frame'
treatmentInfo(object) <- value</pre>
## S4 method for signature 'CoreSet'
```

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```
treatmentNames(object)
## S4 replacement method for signature 'CoreSet, character'
treatmentNames(object) <- value</pre>
## S4 method for signature 'CoreSet'
curation(object)
## S4 replacement method for signature 'CoreSet,list'
curation(object) <- value</pre>
## S4 method for signature 'CoreSet'
datasetType(object)
## S4 replacement method for signature 'CoreSet, character'
datasetType(object) <- value</pre>
## S4 method for signature 'CoreSet'
molecularProfiles(object, mDataType, assay)
## S4 replacement method for signature 'CoreSet, character, character, matrix'
molecularProfiles(object, mDataType, assay) <- value</pre>
## S4 replacement method for signature 'CoreSet,character,missing,matrix'
molecularProfiles(object, mDataType, assay) <- value</pre>
## S4 replacement method for signature 'CoreSet,missing,missing,list_OR_MAE'
molecularProfiles(object, mDataType, assay) <- value</pre>
## S4 method for signature 'CoreSet'
featureInfo(object, mDataType)
## S4 replacement method for signature 'CoreSet,character,data.frame'
featureInfo(object, mDataType) <- value</pre>
## S4 method for signature 'CoreSet, character'
phenoInfo(object, mDataType)
## S4 replacement method for signature 'CoreSet, character, data.frame'
phenoInfo(object, mDataType) <- value</pre>
## S4 method for signature 'CoreSet, character'
fNames(object, mDataType)
## S4 replacement method for signature 'CoreSet, character, character'
fNames(object, mDataType) <- value</pre>
## S4 method for signature 'CoreSet'
```

mDataNames(object) ## S4 replacement method for signature 'CoreSet' mDataNames(object) <- value</pre> ## S4 method for signature 'CoreSet' molecularProfilesSlot(object) ## S4 replacement method for signature 'CoreSet,list\_OR\_MAE' molecularProfilesSlot(object) <- value</pre> ## S4 method for signature 'CoreSet' sensitivityInfo(object, dimension, ...) ## S4 replacement method for signature 'CoreSet, data.frame' sensitivityInfo(object, dimension, ...) <- value</pre> ## S4 method for signature 'CoreSet' sensitivityMeasures(object) ## S4 replacement method for signature 'CoreSet, character' sensitivityMeasures(object) <- value</pre> ## S4 method for signature 'CoreSet' sensitivityProfiles(object) ## S4 replacement method for signature 'CoreSet,data.frame' sensitivityProfiles(object) <- value</pre> ## S4 method for signature 'CoreSet' sensitivityRaw(object) ## S4 replacement method for signature 'CoreSet,array' sensitivityRaw(object) <- value</pre> ## S4 method for signature 'CoreSet' treatmentResponse(object) ## S4 replacement method for signature 'CoreSet,list\_OR\_LongTable' treatmentResponse(object) <- value</pre> ## S4 method for signature 'CoreSet' sensNumber(object) ## S4 replacement method for signature 'CoreSet, matrix' sensNumber(object) <- value</pre> ## S4 method for signature 'CoreSet'

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```
pertNumber(object)
## S4 replacement method for signature 'CoreSet,array'
pertNumber(object) <- value</pre>
```

#### **Arguments**

object A CoreSet object.

value See details.

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.
... See details.

#### **Details**

#### @annotation:

**annotation**: A list of CoreSet 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 CoreSet with.

#### @dateCreated:

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

dateCreated<-: Update the 'dateCreated' item in the annotation slot of a CoreSet object. Arguments:</pre>

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

name: character(1) The name of the CoreSet, retreived from the @annotation slot.

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

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

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

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

• value: a data.frame object.

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

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

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

treatmentInfo: data.frame Metadata for all treatments in a CoreSet object. Arguments:

• object: CoreSet An object to retrieve treatment metadata from.

treatmentInfo<-: CoreSet object with updated treatment metadata. object. Arguments:

- object: CoreSet 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 CoreSet object. Arguments:

• object: CoreSet An object to retrieve treatment names from.

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

- object: CoreSet An object to set treatment names from.
- value: character A character vector of updated treatment names.

#### @curation:

**curation**: A list of curated mappings between identifiers in the CoreSet object and the original data publication. Contains two data.frames, 'sample' with sample ids and 'tissue' with tissue ids.

**curation<-**: Update the curation slot of a CoreSet object. Arugments:

• value: A list of data. frames, one for each type of curated identifier. For a CoreSet object the slot should contain tissue and sample 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 CoreSet 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 CoreSet 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 CoreSet 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 CoreSet 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 CoreSet 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 CoreSet object. More specifically, retrieve the @rowData slot from the SummarizedExperiment from the @molecularProfiles of a CoreSet 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 CoreSet object.

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

**phenoInfo<-**: Update the @colData slot of the SummarizedExperiment of mDataType in the @molecularProfiles slot of a CoreSet 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 CoreSet object.

**fNames**: Updates the rownames of the feature metadata (i.e., rowData) for a SummarizedExperiment of mDataType within a CoreSet object.

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

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

mDataNames: character Retrieve the names of the molecular data types available in the molecularProfiles slot of a CoreSet 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 CoreSet object. Arguments:

olecular Profiles Slot. Return the contents of the amolecular Profiles slot of a CoreSet object

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

**molecularProfilesSlot<-**: Update the contents of the @molecularProfiles slot of a CoreSet 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 CoreSet @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 CoreSet object. When the dimension parameter is used, it allows retrieval of the dimension specific metadata from the LongTable object in @treatmentResponse of a CoreSet object.

**sensitivityInfo<-**: Update the @treatmentResponse slot metadata for a CoreSet object. When used without the dimension argument is behaves similar to the old CoreSet 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 CoreSet 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 CoreSet object. Thesee values are the column names of the 'profiles' assay and represent various compued 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 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 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 CoreSet 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 CoreSet.

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 CoreSet 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 CoreSet 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 CoreSet 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 CoreSet 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(clevelandSmall_cSet)
## @annotation
annotation(clevelandSmall_cSet)
annotation(clevelandSmall_cSet) <- annotation(clevelandSmall_cSet)
dateCreated(clevelandSmall_cSet)
## dateCreated
dateCreated(clevelandSmall_cSet) <- date()
name(clevelandSmall_cSet)
name(clevelandSmall_cSet) <- 'new_name'
sampleInfo(clevelandSmall_cSet) <- sampleInfo(clevelandSmall_cSet)
sampleNames(clevelandSmall_cSet) <- sampleNames(clevelandSmall_cSet)
treatmentInfo(clevelandSmall_cSet)</pre>
```

```
treatmentNames(clevelandSmall_cSet)
treatmentNames(clevelandSmall_cSet) <- treatmentNames(clevelandSmall_cSet)</pre>
## curation
curation(clevelandSmall_cSet)
curation(clevelandSmall_cSet) <- curation(clevelandSmall_cSet)</pre>
datasetType(clevelandSmall_cSet)
datasetType(clevelandSmall_cSet) <- 'both'</pre>
# No assay specified
molecularProfiles(clevelandSmall_cSet, 'rna') <- molecularProfiles(clevelandSmall_cSet, 'rna')</pre>
# Specific assay
molecularProfiles(clevelandSmall_cSet, 'rna', 'exprs') <-</pre>
    molecularProfiles(clevelandSmall_cSet, 'rna', 'exprs')
# Replace the whole slot
molecularProfiles(clevelandSmall_cSet) <- molecularProfiles(clevelandSmall_cSet)</pre>
featureInfo(clevelandSmall_cSet, 'rna')
featureInfo(clevelandSmall_cSet, 'rna') <- featureInfo(clevelandSmall_cSet, 'rna')</pre>
phenoInfo(clevelandSmall_cSet, 'rna')
phenoInfo(clevelandSmall_cSet, 'rna') <- phenoInfo(clevelandSmall_cSet, 'rna')</pre>
fNames(clevelandSmall_cSet, 'rna')
fNames(clevelandSmall_cSet, 'rna') <- fNames(clevelandSmall_cSet, 'rna')</pre>
mDataNames(clevelandSmall_cSet)
mDataNames(clevelandSmall_cSet) <- mDataNames(clevelandSmall_cSet)</pre>
molecularProfilesSlot(clevelandSmall_cSet)
molecularProfilesSlot(clevelandSmall_cSet) <- molecularProfilesSlot(clevelandSmall_cSet)</pre>
sensitivityInfo(clevelandSmall_cSet)
sensitivityInfo(clevelandSmall_cSet) <- sensitivityInfo(clevelandSmall_cSet)</pre>
sensitivityMeasures(clevelandSmall_cSet) <- sensitivityMeasures(clevelandSmall_cSet)</pre>
sensitivityMeasures(clevelandSmall_cSet) <- sensitivityMeasures(clevelandSmall_cSet)</pre>
sensitivityProfiles(clevelandSmall_cSet)
```

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```
sensitivityProfiles(clevelandSmall_cSet) <- sensitivityProfiles(clevelandSmall_cSet)
head(sensitivityRaw(clevelandSmall_cSet))
sensitivityRaw(clevelandSmall_cSet) <- sensitivityRaw(clevelandSmall_cSet)
treatmentResponse(clevelandSmall_cSet)
treatmentResponse(clevelandSmall_cSet) <- treatmentResponse(clevelandSmall_cSet)
sensNumber(clevelandSmall_cSet)
sensNumber(clevelandSmall_cSet) <- sensNumber(clevelandSmall_cSet)
pertNumber(clevelandSmall_cSet)</pre>
```

CoreSet-class

CoreSet - A generic data container for molecular profiles and treatment response data

### Description

CoreSet - A generic data container for molecular profiles and treatment response data

#### **Details**

The CoreSet (cSet) class was developed as a superclass for pSets in the PharmacoGx and RadioGx packages to contain the data generated in screens of cancer sample lines for their genetic profile and sensitivities to therapy (Pharmacological or Radiation). This class is meant to be a superclass which is contained within the PharmacoSet (pSet) and RadioSet (rSet) objects exported by PharmacoGx and RadioGx. The format of the data is similar for both pSets and rSets, allowing much of the code to be abstracted into the CoreSet super-class. However, the models involved with quantifying sampleular response to Pharmacological and Radiation therapy are widely different, and extension of the cSet class allows the packages to apply the correct model for the given data.

### Slots

annotation See Slots section.
molecularProfiles See Slots section.
sample See Slots section.
treatment See Slots section.
treatmentResponse See Slots section.
perturbation See Slots section.
curation See Slots section.
datasetType See Slots section.

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### **Slots**

• annotation: A list of annotation data about the CoreSet, 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 or MultiAssayExperiment containing CoreSet object.
- sample: A data.frame containg the annotations for all the samples profiled in the data set, across all molecular data types and treatment response experiments.
- treatment: A data. frame containing the annotations for all treatments in the dataset, including the mandatory 'treatmentid' column to uniquely identify each treatment.
- treatmentResponse: A list or LongTable containing all the data for the treatment response experiment, 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 sample-drug/radiationInfo pair
- perturbation: list containing \$n, a data. frame summarizing the available perturbation data. This slot is currently being deprecated.
- curation: list containing mappings for treatment, sample and tissue names used in the data set to universal identifiers used between different CoreSet objects.
- datasetType: character string of 'sensitivity', 'perturbation', or both detailing what type of data can be found in the CoreSet, for proper processing of the data

#### See Also

CoreSet-accessors

CoreSet-utils

Utility methods for a CoreSet object.

## Description

Documentation for utility methods for a CoreSet object, such as set operations like subset and intersect. See @details for information on different types of methods and their implementations.

## Usage

```
## S4 method for signature 'CoreSet'
subsetBySample(x, samples)
## S4 method for signature 'CoreSet'
subsetByTreatment(x, treatments)
## S4 method for signature 'CoreSet'
subsetByFeature(x, features, mDataTypes)
```

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#### **Arguments**

x A CoreSet object.

samples character() vector of sample names. Must be valid rownames from sampleInfo(x).

treatments character() vector of treatment names. Must be valid rownames from treatmentInfo(x).

This method does not work with CoreSet objects yet.

features character() vector of feature names. Must be valid feature names for a given

mDataType

mDataTypes character() One or more molecular data types to to subset features by. Must

be valid rownames for the selected SummarizedExperiment mDataTypes.

#### **Details**

#### subset methods:

subsetBySample: Subset a CoreSet object by sample identifier.

• value: a CoreSet object containing only samples.

#### subset methods:

**subsetByTreatment**: Subset a CoreSet object by treatment identifier.

• value: a CoreSet object containing only treatments.

#### subset methods:

subsetByFeature: Subset a CoreSet object by molecular feature identifier.

• value: a CoreSet object containing only features.

#### Value

See details.

## **Examples**

```
data(clevelandSmall_cSet)
## subset methods
### subsetBySample
samples <- sampleInfo(clevelandSmall_cSet)$sampleid[seq_len(10)]
clevelandSmall_cSet_sub <- subsetBySample(clevelandSmall_cSet, samples)

## subset methods
### subsetByTreatment
#treatments <- treatmentInfo(clevelandSmall_cSet)$treatmentid[seq_len(10)]
#clevelandSmall_cSet_sub <- subsetByTreatment(clevelandSmall_cSet, treatments)
## subset methods</pre>
```

CoreSet2 45

```
### subsetByFeature
features <- fNames(clevelandSmall_cSet, 'rna')[seq_len(5)]
clevelandSmall_cSet_sub <- subsetByFeature(clevelandSmall_cSet, features, 'rna')</pre>
```

CoreSet2

Make a CoreSet with the updated class structure

## Description

New implementation of the CoreSet constructor to support MAE and TRE. This constructor will be swapped with the original CoreSet constructor as part of an overhaul of the CoreSet class structure.

### Usage

```
CoreSet2(
  name = "emptySet",
  treatment = data.frame(),
  sample = data.frame(),
  molecularProfiles = MultiAssayExperiment(),
  treatmentResponse = LongTable(),
  datasetType = "sensitivity",
  perturbation = list(n = array(dim = 3), info = "No perturbation data!"),
  curation = list(sample = data.frame(), treatment = data.frame())
)
```

#### **Arguments**

name A character(1) vector with the CoreSet objects name.

treatment A data. frame with treatment level metadata.

sample A data. frame with sample level metadata for the union of samples in treatmentResponse

and molecular Profiles.

molecularProfiles

 $\label{thm:containing} A \; {\tt MultiAssayExperiment} \; containing \; one \; {\tt SummarizedExperiment} \; object \; for \;$ 

each molecular data type.

treatmentResponse

A LongTable or LongTableDataMapper object containing all treatment response

data associated with the CoreSet object.

datasetType A deprecated slot in a CoreSet object included for backwards compatibility.

This may be removed in future releases.

perturbation A deprecated slot in a CoreSet object included for backwards compatibility.

This may be removed in future releases.

curation A list(2) object with two items named treatment and sample with mappings

from publication identifiers to standardized identifiers for both annotations, re-

spectively.

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## Value

A CoreSet object storing standardized and curated treatment response and multiomic profile data associated with a given publication.

## **Examples**

```
data(clevelandSmall_cSet)
clevelandSmall_cSet
```

cosinePerm

Cosine Permutations

## Description

Computes the cosine similarity and significance using permutation test. This function uses random numbers, to ensure reproducibility please call set.seed() before running the function.

## Usage

```
cosinePerm(
    x,
    y,
    nperm = 1000,
    alternative = c("two.sided", "less", "greater"),
    include.perm = FALSE,
    nthread = 1,
    ...
)
```

## Arguments

X	factor is the factors for the first variable
У	factor is the factors for the second variable
nperm	integer is the number of permutations to compute the null distribution of MCC estimates $$
alternative	string indicates the alternative hypothesis and must be one of ''two.sided'', ''greater'' or ''less''. You can specify just the initial letter. ''greater'' corresponds to positive association, ''less'' to negative association. Options are 'two.sided', 'less', or 'greater'
include.perm	boolean indicates whether the estimates for the null distribution should be returned. Default set to 'FALSE'
nthread	integer is the number of threads to be used to perform the permutations in parallel $% \left( 1\right) =\left( 1\right) \left( 1$
	A list of fallthrough parameters

DataMapper-accessors

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#### Value

A list estimate of the cosine similarity, p-value and estimates after random permutations (null distribution) in include.perm is set to 'TRUE'

### **Examples**

```
x <- factor(c(1,2,1,2,1))
y <- factor(c(2,2,1,1,1))
cosinePerm(x, y)</pre>
```

DataMapper-accessors Accessing and modifying data in a DataMapper object.

#### Description

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

### Usage

```
## S4 method for signature 'DataMapper'
rawdata(object)
## S4 replacement method for signature 'DataMapper,ANY'
rawdata(object) <- value</pre>
```

### **Arguments**

object A DataMapper object to get or set data from.

value A list-like object to assign to the rawdata slot. Should be a data.frame or

data.table with the current implementation.

## **Details**

**rawdata**: Get the raw data slot from a DataMapper object. Returns a list-like containing one or more raw data inputs to the DataMapper object.

rawdata: Set the raw data slot from a DataMapper object. value: The list-like object to set for the rawdata slot. Note: this currently only supports data. frame or data. table objects.

## Value

Accessors: See details

Setters: An update DataMapper object, returned invisibly.

### See Also

Other DataMapper-accessors: LongTableDataMapper-accessors, TREDataMapper-accessors

drop\_fn\_params

DataMapper-class	An S4 Class For Mapping from Raw Experimental Data to a Specific S4 Object

## **Description**

This object will be used as a way to abstract away data preprocessing.

#### **Slots**

- rawdata: A list-like object containing one or more pieces of raw data that will be processed and mapped to the slots of an S4 object.
- metadata: A List of object level metadata.

drop_fn_params	Drop parameters from a function and replace them with constants inside the function body.
	, , , , , , , , , , , , , , , , , , ,

## Description

Drop parameters from a function and replace them with constants inside the function body.

## Usage

```
drop_fn_params(fn, args)
```

## **Arguments**

fn	function A non-primitive function to remove parameters from (via base::formals(fn)).

args list A list where names are the function arguments (parameters) to remove and

the values are the appopriate value to replace the parameter with in the function

body.

## Value

function A new non-primitize function with the parameters named in args deleted and their values fixed with the values from args in the function body.

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endoaggregate

Perform aggregation over an S4 object, but return an object of the same class.

## Description

Perform aggregation over an S4 object, but return an object of the same class.

## Usage

```
endoaggregate(x, ...)
```

## Arguments

x An S4 object to endomorphically aggregate over.

... pairlist Allow definition of new parameters for implementations of this generic.

#### Value

An object with the same class as x.

### **Examples**

```
print("Generics shouldn't need examples?")
```

```
endoaggregate,LongTable-method
```

Functional API for endomorphic aggregation over a LongTable or inheriting class

## **Description**

Compute a group-by operation over a LongTable object or its inhering classes.

## Usage

```
## S4 method for signature 'LongTable'
endoaggregate(
    x,
    ...,
    assay,
    target = assay,
    by,
    subset = TRUE,
    nthread = 1,
```

```
progress = TRUE,
BPPARAM = NULL,
enlist = TRUE,
moreArgs = list()
```

### **Arguments**

x LongTable or inheriting class to compute aggregation on.

... call One or more aggregations to compute for each group by in x. If you name aggregation calls, that will be the column name of the value in the resulting data.table otherwise a default name will be parsed from the function name and its first argument, which is assumed to be the name of the column being

aggregated over.

assay character(1) The assay to aggregate over.

target character(1) The assay to assign the results to. Defaults to assay.

by character One or more valid column names in x to compute groups using.

subset call An R call to evaluate before perfoming an aggregate. This allows you to

aggregate over a subset of columns in an assay but have it be assigned to the parent object. Default is TRUE, which includes all rows. Passed through as the

i argument in [.data.table.

nthread numeric(1) Number of threads to use for split-apply-combine parallelization.

Uses BiocParllel::bplapply if nthread > 1 or you pass in BPPARAM. Does not modify data.table threads, so be sure to use setDTthreads for reasonable nested

parallelism. See details for performance considerations.

progress logical(1) Display a progress bar for parallelized computations? Only works

if bpprogressbar<- is defined for the current BiocParallel back-end.

BPPARAM BiocParallelParam object. Use to customized the the parallization back-end

of bplapply. Note, nthread over-rides any settings from BPPARAM as long as

bpworkers<- is defined for that class.

enlist logical(1) Default is TRUE. Set to FALSE to evaluate the first call in . . . within

data.table groups. See details for more information.

moreArgs list() A named list where each item is an argument one of the calls in ...

which is not a column in the table being aggregated. Use to further parameterize you calls. Please note that these are not added to your aggregate calls unless you

specify the names in the call.

### **Details**

### **Use of Non-Standard Evaluation:**

Arguments in . . . are substituted and wrapped in a list, which is passed through to the j argument of [.data.table internally. The function currently tries to build informative column names for unnamed arguments in . . . by appending the name of each function call with the name of its first argument, which is assumed to be the column name being aggregated over. If an argument to . . . is named, that will be the column name of its value in the resulting data.table.

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### **Enlisting:**

The primary use case for enlist=FALSE is to allow computation of dependent aggregations, where the output from a previous aggregation is required in a subsequent one. For this case, wrap your call in { and assign intermediate results to variables, returning the final results as a list where each list item will become a column in the final table with the corresponding name. Name inference is disabled for this case, since it is assumed you will name the returned list items appropriately. A major advantage over multiple calls to aggregate is that the overhead of parallelization is paid only once even for complex multi-step computations like fitting a model, capturing its paramters, and making predictions using it. It also allows capturing arbitrarily complex calls which can be recomputed later using the update, TreatmentResponseExperiment-method A potential disadvantage is increased RAM usage per thread due to storing intermediate values in variables, as well as any memory allocation overhead associate therewith.

#### Value

Object with the same class as x, with the aggregation results assigned to target, using strategy if target is an existing assay in x.

### See Also

```
data.table::[.data.table, BiocParallel::bplapply
```

exampleDataMapper

Example LongTableDataMapper

### **Description**

A dummy LongTableDataMapper object to be used in package examples.

## Usage

data(exampleDataMapper)

### **Format**

LongTableDataMapper object

52 guessMapping

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Retrieve the specified item from object internal metadata.

## **Description**

Internal slot for storing metadata relevant to the internal operation of an S4 object.

## Usage

```
getIntern(object, x, ...)
```

## Arguments

object S4 An object with an @.itern slot containing an environment.

x character One or more symbol names to retrieve from the object@.intern en-

vironment.

... Allow new parmeters to be defined for this generic.

## **Details**

Warning: This method is intended for developer use and can be ignored by users.

## Value

Depends on the implemented method

## **Examples**

```
print("Generics shouldn't need examples?")
```

guessMapping

Generic for Guessing the Mapping Between Some Raw Data and an S4 Object

## **Description**

Generic for Guessing the Mapping Between Some Raw Data and an S4 Object

## Usage

```
guessMapping(object, ...)
```

#### **Arguments**

object An S4 object containing so raw data to guess data to object slot mappings for.

... Allow new arguments to be defined for this generic.

#### Value

A list with mapping guesses as items.

### **Examples**

"Generics shouldn't need examples!"

guessMapping,LongTableDataMapper-method

Guess which columns in raw experiment data map to which dimensions.

## Description

Checks for columns which are uniquely identified by a group of identifiers. This should be used to help identify the columns required to uniquely identify the rows, columns, assays and metadata of a DataMapper class object.

## Usage

```
## S4 method for signature 'LongTableDataMapper'
guessMapping(object, groups, subset, data = FALSE)
```

## **Arguments**

object	A LongTableDataMapper object.

groups A list containing one or more vector of column names to group-by. The func-

tion uses these to determine 1:1 mappings between the combination of columns

in each vector and unique values in the raw data columns.

subset A logical vector indicating whether to to subset out mapped columns after each

grouping. Must be a single TRUE or FALSE or have the same length as groups, indicating whether to subset out mapped columns after each grouping. This will

prevent mapping a column to two different groups.

data A logical vector indicating whether you would like the data for mapped columns

to be returned instead of their column names. Defaults to FALSE for easy use as-

signing mapped columns to a DataMapper object.

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## **Details**

Any unmapped columns will be added to the end of the returned list in an item called unmapped. The function automatically guesses metadata by checking if any columns have only a single value. This is returned as an additional item in the list.

## Value

A list, where each item is named for the associated groups item the guess is for. The character vector in each item are columns which are uniquely identified by the identifiers from that group.

## **Examples**

```
guessMapping(exampleDataMapper, groups=list(rows='treatmentid', cols='sampleid'),
subset=FALSE)
```

gwc

**GWC Score** 

## **Description**

Calculate the gwc score between two vectors, using either a weighted spearman or pearson correlation

## Usage

```
gwc(
    x1,
    p1,
    x2,
    p2,
    method.cor = c("pearson", "spearman"),
    nperm = 10000,
    truncate.p = 1e-16,
    ...
)
```

### **Arguments**

x1	numeric vector of effect sizes (e.g., fold change or t statitsics) for the first experiment
p1	numeric vector of p-values for each corresponding effect size for the first experiment
x2	numeric effect size (e.g., fold change or t statitsics) for the second experiment
p2	numeric vector of p-values for each corresponding effect size for the second experiment

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method.cor character string identifying if a pearson or spearman correlation should be used

nperm numeric how many permutations should be done to determine

truncate.p numeric Truncation value for extremely low p-values

Other passed down to internal functions

### Value

numeric a vector of two values, the correlation and associated p-value.

## **Examples**

```
data(clevelandSmall_cSet)
x <- molecularProfiles(clevelandSmall_cSet,'rna')[,1]
y <- molecularProfiles(clevelandSmall_cSet,'rna')[,2]
x_p <- rep(0.05, times=length(x))
y_p <- rep(0.05, times=length(y))
names(x_p) <- names(x)
names(y_p) <- names(y)
gwc(x,x_p,y,y_p, nperm=100)</pre>
```

idCols

Generic to access the unique id columns in an S4 object used to

## **Description**

Generic to access the unique id columns in an S4 object used to

#### Usage

```
idCols(object, ...)
```

### **Arguments**

object An S4 object to get id columns from.
... Allow new arguments to this generic.

## Value

Depends on the implemented method

## **Examples**

```
print("Generics shouldn't need examples?")
```

56 immutable

immutable

Constructor for "immutable" S3-class property

## **Description**

This method should allow any S3 object in R to become immutable by intercepting [<-, [[<-, \$<- and c during S3-method dispatch and returning an error.

Reverse with call to the mutable function.

### Usage

```
immutable(object)
is.immutable(object)
## S3 method for class 'immutable'
print(x, ...)
show.immutable(x)
```

### **Arguments**

```
object, x Any R object which uses S3 method dispatch
... Fallthrough arguments to print.default.
```

### **Details**

The motivation for this class was to create pseudo-private slots in an R S4 object by preventing mutation of those slots outside of the accessors written for the class. It should behave as expected for R object which operate with 'copy-on-modify' semantics, including most base R functions and S3 objects.

An environment was not suitable for this case due to the 'copy-by-reference' semantics, such that normal R assignment, which users assume makes a copy of the object, actually references the same environment in both the original and copy of the object.

WARNING: This implementation is unable to intercept modifications to a data.table via the set\* group of methods. This is because these methods are not S3 generics and therefore no mechanism exists for hooking into them to extend their functionality. In general, this helper class will only work for objects with an S3 interface.

### Value

```
The object with "immutable" prepended to its class attribute.

logical(1) Does the object inherit from the "immutable" S3-class?

None, invisible(NULL)
```

is.items 57

### See Also

```
assignment-immutable, setOps-immutable
```

## **Examples**

```
immutable_list <- immutable(as.list(1:5))
class(immutable_list)
# errors during assignment operations
tryCatch({ immutable_list$new <- 1 }, error=print)
immutable_list <- immutable(as.list(1:5))
is.immutable(immutable_list)</pre>
```

is.items

Get the types of all items in a list

## **Description**

Get the types of all items in a list

### Usage

```
is.items(list, ..., FUN = is)
```

### **Arguments**

list A list to get the types from

... pairlist Additional arguments to FUN

FUN function or character Either a function, or the name of a function which

returns a single logical value. The default function uses is, specify the desired type in . . . . You can also use other type checking functions such as is.character,

is.numeric, or is.data.frame.

### Value

logical A vector indicating if the list item is the specified type.

## **Examples**

```
list <- list(c(1,2,3), c('a','b','c'))
is.items(list, 'character')</pre>
```

 $\begin{tabular}{lll} is \verb| optim| compatible & Check whether a function signature is amenable to optimization via \\ & stats::optim. \end{tabular}$ 

## **Description**

Functions compatible with optim have the parameter named par as their first formal argument where each value is a respective free parameter to be optimized.

### Usage

```
is_optim_compatible(fn)
```

## Arguments

fn function A non-primitive function.

### Value

logical(1) TRUE if the first value of formalArg(fn) is "par", otherwise FALSE.

```
lapply\,, \verb|MultiAssay| Experiment-method|\\ lapply\,lapply\,method\,for\, \verb|MultiAssay| Experiment|
```

## Description

lapply lapply method for MultiAssayExperiment

## Usage

```
## S4 method for signature 'MultiAssayExperiment'
lapply(X, FUN, ...)
```

### **Arguments**

X A MultiAssayExperiment object.

FUN A function to be applied to each SummarizedExperiment in a in X.

... Fall through parameters to FUN

### Value

```
A MultiAssayExperiment object, modifed such that experiments(X) <- endoapply(experiments(X), FUN, ...).s
```

```
list_OR_LongTable-class
```

A class union to allow multiple types in a CoreSet slot

## Description

A class union to allow multiple types in a CoreSet slot

LongTable

 $Long Table\ constructor\ method$ 

## Description

LongTable constructor method

## Usage

```
LongTable(
  rowData,
  rowIDs,
  colData,
  colIDs,
  assays,
  assayIDs,
  metadata = list(),
  keep.rownames = FALSE
)
```

## **Arguments**

rowData	data.frame A rectangular object coercible to a data.table.
rowIDs	character A vector of rowData column names needed to uniquely identify each row in a LongTable. \\\\
colData	data.frame A rectangular object coercible to a data.table.
colIDs	chacter A vector of colData column names needed to uniquely identify each column in a $LongTable$ .
assays	list A list of rectangular objects, each coercible to a data.table. Must be named and item names must match the assayIDs list.
assayIDs	list A list of character vectors specifying the columns needed to uniquely identify each row in an assay. Names must match the assays list.
metadata	list A list of one or more metadata items associated with a LongTable experiment.
keep.rownames	logical(1) or character(1) Should rownames be retained when coercing to data.table inside the constructor. Default is FALSE. If TRUE, adds a 'rn' column to each rectangular object that gets coerced from data.frame to data.table. If a string, that becomes the name of the rownames column.

### Value

A LongTable object containing the data for a treatment response experiment and configured according to the rowIDs and colIDs arguments.

### **Examples**

```
"See vignette('The LongTable Class', package='CoreGx')"
```

LongTable-accessors

Accessing and modifying information in a LongTable

## **Description**

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

#### Value

Accessors: See details.

Setters: An updated LongTable object, returned invisibly.

### **Examples**

```
data(merckLongTable)
```

LongTableDataMapper

Constructor for the LongTableDataMapper class, which maps from one or more raw experimental data files to the slots of a LongTable object.

## **Description**

Constructor for the LongTableDataMapper class, which maps from one or more raw experimental data files to the slots of a LongTable object.

## Usage

```
LongTableDataMapper(
  rawdata = data.frame(),
  rowDataMap = list(character(), character()),
  colDataMap = list(character(), character()),
  assayMap = list(list(character(), character())),
  metadataMap = list(character())
```

#### **Arguments**

rawdata A data.frame of raw data from a treatment response experiment. This will be

coerced to a data.table internally. We recommend using joins to aggregate

your raw data if it is not present in a single file.

rowDataMap A list-like object containing two character vectors. The first is column names

in rawdata needed to uniquely identify each row, the second is additional columns which map to rows, but are not required to uniquely identify them. Rows should

be drugs.

colDataMap A list-like object containing two character vectors. The first is column names

in rawdata needed to uniquely identify each column, the second is additional columns which map to rows, but are not required to uniquely identify them.

Columns should be samples.

assayMap A list-like where each item is a list with two character vectors defining an

assay, the first containing the identifier columns in rawdata needed to uniquely identify each row an assay, and the second the rawdata columns to be mapped to that assay. The names of assayMap will be the names of the assays in the LongTable that is created when calling metaConstruct on this DataMapper object. If the character vectors have names, the value columns will be renamed

accordingly.

metadataMap A list-like where each item is a character vector of rawdata column names to

assign to the @metadata of the LongTable, where the name of that assay is the name of the list item. If names are omitted, assays will be numbered by their

index in the list.

### Details

The guessMapping method can be used to test hypotheses about the cardinality of one or more sets of identifier columns. This is helpful to determine the id columns for rowDataMap and colDataMap, as well as identify columns mapping to assays or metadata.

To attach metadata not associated with rawdata, please use the metadata assignment method on your LongTableDataMapper. This metadata will be merged with any metadata from metadataMap and added to the LongTable which this object ultimately constructs.

### Value

A LongTable object, with columns mapped to it's slots according to the various maps in the LongTableDataMapper object.

#### See Also

guessMapping

#### **Examples**

data(exampleDataMapper)
exampleDataMapper

LongTableDataMapper-accessors

Accessing and modifying data in a LongTableDataMapper object.

#### **Description**

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

## Usage

```
## S4 replacement method for signature 'LongTableDataMapper,list'
rawdata(object) <- value</pre>
## S4 method for signature 'LongTableDataMapper'
rowDataMap(object)
## S4 replacement method for signature 'LongTableDataMapper,list_OR_List'
rowDataMap(object) <- value</pre>
## S4 method for signature 'LongTableDataMapper'
colDataMap(object)
## S4 replacement method for signature 'LongTableDataMapper,list_OR_List'
colDataMap(object) <- value</pre>
## S4 method for signature 'LongTableDataMapper'
assayMap(object)
## S4 replacement method for signature 'LongTableDataMapper,list_OR_List'
assayMap(object) <- value</pre>
## S4 method for signature 'LongTableDataMapper'
metadataMap(object)
## S4 replacement method for signature 'LongTableDataMapper,list_OR_List'
metadataMap(object) <- value</pre>
```

### **Arguments**

object A LongTableDataMapper object to get or set data from. value See details.

### Details

**rawdata**: Get the raw data slot from a LongTableDataMapper object. Returns a list-like containing one or more raw data inputs to the LongTableDataMapper object.

**rawdata**: Set the raw data slot from a LongTableDataMapper object. **value**: The list-like object to set for the rawdata slot. Note: this currently only supports data.frame or data.table objects.

**rowDataMap**: list of two character vectors, the first are the columns required to uniquely identify each row of a LongTableDataMapper and the second any additional row-level metadata. If the character vectors have names, the resulting columns are automatically renamed to the item name of the specified column.

**rowDataMap<-**: Update the @rowDataMap slot of a LongTableDataMapper object, returning an invisible NULL. Arguments:

• value: A list or List where the first item is the names of the identifier columns – columns needed to uniquely identify each row in rowData – and the second item is the metadata associated with those the identifier columns, but not required to uniquely identify rows in the object rowData.

**colDataMap**: list of two character vectors, the first are the columns required to uniquely identify each row of a LongTableDataMapper and the second any additional col-level metadata. If the character vectors have names, the resulting columns are automatically renamed to the item name of the specified column.

colDataMap<-: Update the @colDataMap slot of a LongTableDataMapper object, returning an invisible NULL. Arguments:

• value: A list or List where the first item is the names of the identifier columns – columns needed to uniquely identify each row in colData – and the second item is the metadata associated with those the identifier columns, but not required to uniquely identify rows in the object rowData.

**assayMap**: A list of character vectors. The name of each list item will be the assay in a LongTableDataMapper object that the columns in the character vector will be assigned to. Column renaming occurs automatically when the character vectors have names (from the value to the name).

**assayMap<-**: Updates the @assayMap slot of a LongTableDataMapper object, returning an invisible NULL. Arguments:

value: A list of character vectors, where the name of each list item is the name of an assay
and the values of each character vector specify the columns mapping to the assay in the S4
object the LongTableDataMapper constructs.

**metadataMap**: A list of character vectors. Each item is an element of the constructed objects @metadata slot.

**metadataMap<-**: Updates LongTableDataMapper object in-place, then returns an invisible(NULL). Arguments:

 value: A list of character vectors. The name of each list item is the name of the item in the @metadata slot of the LongTableDataMapper object created when metaConstruct is called on the DataMapper, and a character vector specifies the columns of @rawdata to assign to each item.

#### Value

Accessors: See details

Setters: An update LongTableDataMapper object, returned invisibly.

### See Also

Other DataMapper-accessors: DataMapper-accessors, TREDataMapper-accessors

### **Examples**

```
rowDataMap(exampleDataMapper)
rowDataMap(exampleDataMapper) <- list(c('treatmentid'), c())
colDataMap(exampleDataMapper)
colDataMap(exampleDataMapper) <- list(c('sampleid'), c())
assayMap(exampleDataMapper)
assayMap(exampleDataMapper) <- list(sensitivity=c(viability1='viability'))
metadataMap(exampleDataMapper)
metadataMap(exampleDataMapper) <- list(object_metadata=c('metadata'))</pre>
```

LongTableDataMapper-class

A Class for Mapping Between Raw Data and an LongTable Object

## Description

A Class for Mapping Between Raw Data and an LongTable Object

## Usage

```
## S4 method for signature 'LongTableDataMapper'
show(object)
```

### **Arguments**

object

A LongTableDataMapper to display in the console.

### Value

invisible Prints to console.

## **Functions**

• show(LongTableDataMapper): Show method for LongTableDataMapper. Determines how the object is displayed in the console.

make\_optim\_function 65

#### Slots

```
rawdata See Slots section.
rowDataMap See Slots section.
colDataMap See Slots section.
assayMap See Slots section.
metadataMap See Slots section.
```

### **Slots**

- rowDataMap: A list-like object containing two character vectors. The first is column names in rawdata needed to uniquely identify each row, the second is additional columns which map to rows, but are not required to uniquely identify them. Rows should be drugs.
- colDataMap: A list-like object containing two character vectors. The first is column names in rawdata needed to uniquely identify each column, the second is additional columns which map to rows, but are not required to uniquely identify them. Columns should be samples.
- assayMap A list-like where each item is a list with two elements specifying an assay, the
  first being the identifier columns in rawdata needed to uniquely identify each row an assay,
  and the second a list of rawdata columns to be mapped to that assay. The names of assayMap
  will be the names of the assays in the LongTable that is created when calling metaConstruct
  on this DataMapper object.
- metadataMap: A list-like where each item is a character vector of rawdata column names to assign to the @metadata of the LongTable, where the name of that assay is the name of the list item. If names are omitted, assays will be numbered by their index in the list.
- rawdata: A list-like object containing one or more pieces of raw data that will be processed and mapped to the slots of an S4 object.
- metadata: A List of object level metadata.

#### **Examples**

```
show(exampleDataMapper)
```

make\_optim\_function

Takes a non-primitive R function and refactors it to be compatible with optimization via stats::optim.

#### **Description**

Takes a non-primitive R function and refactors it to be compatible with optimization via stats::optim.

### Usage

```
make_optim_function(fn, ...)
```

66 mcc

#### **Arguments**

fn function A non-primitive function

... Arguments to fn to fix for before building the function to be optimized. Useful for reducing the number of free parameters in an optimization if there are

insufficient degrees of freedom.

#### See Also

```
drop_fn_params, collect_fn_params
```

mcc

Compute a Mathews Correlation Coefficient

### Description

The function computes a Matthews correlation coefficient for two factors provided to the function. It assumes each factor is a factor of class labels, and the enteries are paired in order of the vectors.

### Usage

```
mcc(
    x,
    y,
    nperm = 1000,
    nthread = 1,
    alternative = c("two.sided", "less", "greater"),
    ...
)
```

### **Arguments**

x, y factor of the same length with the same number of levels

nperm numeric number of permutations for significance estimation. If 0, no permuta-

tion testing is done

nthread numeric can parallelize permutation texting using BiocParallels bplapply

alternative indicates the alternative hypothesis and must be one of "two.sided", "greater"?

or "less". You can specify just the initial letter. "greater" corresponds to

positive association, "less" to negative association.

... list Additional arguments

## Details

Please note: we recommend you call set.seed() before using this function to ensure the reproducibility of your results. Write down the seed number or save it in a script if you intend to use the results in a publication.

merckLongTable 67

## Value

A list with the MCC as the \$estimate, and p value as \$p.value

## **Examples**

```
x <- factor(c(1,2,1,2,3,1))
y <- factor(c(2,1,1,1,2,2))
mcc(x,y)</pre>
```

merckLongTable

Merck Drug Combination Data LongTable

## Description

This is a LongTable object created from some drug combination data provided to our lab by Merck.

## Usage

```
data(merckLongTable)
```

### **Format**

LongTable object

### References

TODO:: Include a reference

mergeAssays

Merge assays with an S4 object.

## **Description**

Merge assays with an S4 object.

## Usage

```
mergeAssays(object, ...)
```

## Arguments

object S4 An S4 object a list-like slot containing assays for the object.

... Allow new arguments to be defined for this generic.

### Value

A modified version of object.

## **Examples**

```
"This is a generic method!"
```

mergeAssays,LongTable-method

Endomorphically merge assays within a LongTable or inheriting class

## Description

Endomorphically merge assays within a LongTable or inheriting class

## Usage

```
## S4 method for signature 'LongTable'
mergeAssays(object, x, y, target = x, ..., metadata = FALSE)
```

### Arguments

object	A LongTable or inheriting class.
X	character(1) A valid assay name in object.
У	character(1) A valid assay name in object.
target	character(1) Name of the assay to assign the result to. Can be a new or existing assay. Defaults to x.

Fallthrough arguments to merge.data.table to specify the join type. Use this to

 $specify\ which\ columns\ to\ merge\ on.\ If\ excluded,\ defaults\ to\ by=assay Keys (objecty,$ 

y).

metadata logical A logical vector indicating whether to attach metadata to either assay

before the merge occurs. If only one value is passed that value is used for both

assays. Defaults to FALSE.

### Value

A copy of object with assays x and y merged and assigned to target.

### Author(s)

Christopher Eeles

### See Also

```
merge.data.table
```

metaConstruct 69

metaConstruct	Generic for preprocessing complex data before being used in the constructor of an S4 container object.

#### **Description**

This method is intended to abstract away complex constructor arguments and data preprocessing steps needed to transform raw data, such as that produced in a treatment-response or next-gen sequencing experiment, and automate building of the appropriate S4 container object. This is intended to allow mapping between different experimental designs, in the form of an S4 configuration object, and various S4 class containers in the Bioconductor community and beyond.

## Usage

```
metaConstruct(mapper, ...)
## S4 method for signature 'LongTableDataMapper'
metaConstruct(mapper)
## S4 method for signature 'TREDataMapper'
metaConstruct(mapper)
```

### **Arguments**

mapper An TREDataMapper object abstracting arguments to an the TreatmentResponseExperiment constructor.

Allow new arguments to be defined for this generic.

### Value

An S4 object for which the class corresponds to the type of the build configuration object passed to this method.

A LongTable object, as specified in the mapper.

A TreatmentResponseExperiment object, as specified in the mapper.

### **Examples**

```
data(exampleDataMapper)
rowDataMap(exampleDataMapper) <- list(c('treatmentid'), c())
colDataMap(exampleDataMapper) <- list(c('sampleid'), c())
assayMap(exampleDataMapper) <- list(sensitivity=list(c("treatmentid", "sampleid"), c('viability')))
metadataMap(exampleDataMapper) <- list(experiment_metadata=c('metadata'))
longTable <- metaConstruct(exampleDataMapper)
longTable

data(exampleDataMapper)
exampleDataMapper <- as(exampleDataMapper, "TREDataMapper")</pre>
```

```
rowDataMap(exampleDataMapper) <- list(c('treatmentid'), c())</pre>
colDataMap(exampleDataMapper) <- list(c('sampleid'), c())</pre>
assayMap(exampleDataMapper) <- list(sensitivity=list(c("treatmentid", "sampleid"), c('viability')))\\
metadataMap(exampleDataMapper) <- list(experiment_metadata=c('metadata'))</pre>
tre <- metaConstruct(exampleDataMapper)</pre>
```

metadata,LongTable-method

Getter method for the metadata slot of a LongTable object

### **Description**

Getter method for the metadata slot of a LongTable object

## Usage

```
## S4 method for signature 'LongTable'
metadata(x)
```

# **Arguments** Х

The LongTable object from which to retrieve the metadata list.

### Value

list The contents of the metadata slot of the LongTable object.

```
metadata<-,LongTable-method
```

Setter method for the metadata slot of a LongTable object

## Description

Setter method for the metadata slot of a LongTable object

### Usage

```
## S4 replacement method for signature 'LongTable'
metadata(x) \leftarrow value
```

## **Arguments**

LongTable The LongTable to update Χ

value list A list of new metadata associated with a LongTable object. mutable 71

## Value

LongTable A copy of the LongTable object with the value in the metadata slot.

mutable

Remove the "immutable" S3-class from an R object, allowing it to be modified normally again.

## **Description**

Remove the "immutable" S3-class from an R object, allowing it to be modified normally again.

## Usage

```
mutable(object)
```

### **Arguments**

object

An R object inheriting from the "immutable" class.

### Value

The object with the "immutable" class stripped from it.

### **Examples**

```
immut_list <- immutable(list())
mutable(immut_list)</pre>
```

nci\_TRE\_small

NCI-ALMANAC Drug Combination Data TreatmentResponseExperiment Subset

## Description

This is a TreatmentResponseExperiment object containing a subset of NCI-ALMANAC drug combination screening data, with 2347 unique treatment combinations on 10 cancer cell lines selected.

### Usage

```
data(nci_TRE_small)
```

## **Format**

TreatmentResponseExperiment object

72 optimizeCoreGx

### References

Susan L. Holbeck, Richard Camalier, James A. Crowell, Jeevan Prasaad Govindharajulu, Melinda Hollingshead, Lawrence W. Anderson, Eric Polley, Larry Rubinstein, Apurva Srivastava, Deborah Wilsker, Jerry M. Collins, James H. Doroshow; The National Cancer Institute ALMANAC: A Comprehensive Screening Resource for the Detection of Anticancer Drug Pairs with Enhanced Therapeutic Activity. Cancer Res 1 July 2017; 77 (13): 3564–3576. https://doi.org/10.1158/0008-5472.CAN-17-0489

optimizeCoreGx	A helper method to find the best multithreading configuration for your computer
----------------	---

## **Description**

A helper method to find the best multithreading configuration for your computer

### Usage

```
optimizeCoreGx(sample_data, set = FALSE, report = !set)
```

## **Arguments**

sample_data Treat	mentResponseExperiment
-------------------	------------------------

set logical(1) Should the function modify your R environment with the predicted

optimal settings? This changes the global state of your R session!

report logical(1) Should a data. frame of results be returned by number of threads

and operation be returned? Defaults to !set.

### Value

If set=TRUE, modifies data.table threads via setDTthreads(), otherwise displays a message indicating the optimal number of threads. If report=TRUE, also returns a data.frame of the benchmark results.

## **Examples**

```
data(merckLongTable)
optimizeCoreGx(merckLongTable)
```

reindex 73

reindex

Generic method for resetting indexing in an S4 object

# **Description**

This method allows integer indexes used to maintain referential integrity internal to an S4 object to be reset. This is useful particularly after subsetting an object, as certain indexes may no longer be present in the object data. Reindexing removes gaps integer indexes and ensures that the smallest contiguous integer values are used in an objects indexes.

# Usage

```
reindex(object, ...)
```

### **Arguments**

object S4 An object to redo indexing for

... pairlist Allow definition of new parameters to this generic.

### Value

Depends on the implemented method

### **Examples**

```
print("Generics shouldn't need examples?")
```

reindex,LongTable-method

Redo indexing for a LongTable object to remove any gaps in integer indexes

### **Description**

After subsetting a LongTable, it is possible that values of rowKey or colKey could no longer be present in the object. As a result there the indexes will no longer be contiguous integers. This method will calcualte a new set of rowKey and colKey values such that integer indexes are the smallest set of contiguous integers possible for the data.

### Usage

```
## S4 method for signature 'LongTable'
reindex(object)
```

### **Arguments**

object

The LongTable object to recalcualte indexes (rowKey and colKey values) for.

#### Value

A copy of the LongTable with all keys as the smallest set of contiguous integers possible given the current data.

rowData,LongTableDataMapper-method

Convenience method to subset the rowData out of the rawdata slot using the assigned rowDataMap metadata.

# Description

Convenience method to subset the rowData out of the rawdata slot using the assigned rowDataMap metadata.

### Usage

```
## S4 method for signature 'LongTableDataMapper'
rowData(x, key = TRUE)
```

### **Arguments**

x LongTableDataMapper object with valid data in the rawdata and colDataMap

slots.

key logical(1) Should the table be keyed according to the id\_columns of the

rowDataMap slot? This will sort the table in memory. Default is TRUE.

### Value

data.table The rowData as specified in the rowDataMap slot.

rowData,TREDataMapper-method

Convenience method to subset the rowData out of the rawdata slot using the assigned rowDataMap metadata.

### **Description**

Convenience method to subset the rowData out of the rawdata slot using the assigned rowDataMap metadata.

rowIDs 75

# Usage

```
## S4 method for signature 'TREDataMapper'
rowData(x, key = TRUE)
```

# Arguments

x TREDataMapper object with valid data in the rawdata and colDataMap slots.

key logical(1) Should the table be keyed according to the id\_columns of the

rowDataMap slot? This will sort the table in memory. Default is TRUE.

# Value

data.table The rowData as specified in the rowDataMap slot.

rowIDs

Generic to access the row identifiers from

# Description

Generic to access the row identifiers from

# Usage

```
rowIDs(object, ...)
```

# Arguments

object S4 An object to get row id columns from.

... Allow new arguments to this generic.

### Value

Depends on the implemented method.

```
print("Generics shouldn't need examples?")
```

76 sensitivityInfo

rowMeta

Generic to access the row identifiers from

# Description

Generic to access the row identifiers from

# Usage

```
rowMeta(object, ...)
```

# **Arguments**

object S4 An object to get row metadata columns from.

... Allow new arguments to this generic.

### Value

Depends on the implemented method.

### **Examples**

```
print("Generics shouldn't need examples?")
```

sensitivityInfo

Generic function to get the annotations for a treatment response experiment from an S4 class

### **Description**

Generic function to get the annotations for a treatment response experiment from an S4 class

# Usage

```
sensitivityInfo(object, ...)
```

# **Arguments**

object An S4 object to get treatment response experiment annotations from.

... Allow new arguments to be defined for this generic.

# Value

Depends on the implemented method

sensitivityInfo<-

### **Examples**

```
print("Generics shouldn't need examples?")
```

sensitivityInfo<-

sensitivityInfo<- Generic Method

# Description

Generic function to get the annotations for a treatment response experiment from an S4 class.

### Usage

```
sensitivityInfo(object, ...) <- value</pre>
```

# Arguments

object An S4 object to set treatment response experiment annotations for.

... Allow new arguments to be defined for this generic.

value The new treatment response experiment annotations.

### Value

Depends on the implemented method

# **Examples**

```
print("Generics shouldn't need examples?")
```

sensitivityMeasures

sensitivityMeasures Generic

# Description

Get the names of the sensitivity summary metrics available in an S4 object.

# Usage

```
sensitivityMeasures(object, ...)
```

# Arguments

object An S4 object to retrieve the names of sensitivty summary measurements for.

... Fallthrough arguements for defining new methods

sensitivityMeasures<-

# Value

Depends on the implemented method

# **Examples**

```
sensitivityMeasures(clevelandSmall_cSet)
```

```
sensitivityMeasures<- Generic</pre>
```

# Description

Set the names of the sensitivity summary metrics available in an S4 object.

# Usage

```
sensitivityMeasures(object, ...) <- value</pre>
```

# Arguments

object An S4 object to update.

... Allow new methods to be defined for this generic.

value A set of names for sensitivity measures to use to update the object with.

### Value

Depends on the implemented method

```
print("Generics shouldn't need examples?")
```

sensitivityProfiles 79

sensitivityProfiles sensitivityProfiles Generic

### **Description**

A generic for sensitivityProfiles getter method

### Usage

```
sensitivityProfiles(object, ...)
```

# **Arguments**

object The S4 object to retrieve sensitivity profile summaries from.
... pairlist Allow defining new arguments for this generic.

#### Value

Depends on the implemented method

# **Examples**

```
print("Generics shouldn't need examples?")
```

```
sensitivityProfiles<- sensitivityProfiles<- Generic
```

# Description

A generic for the sensitivityProfiles replacement method

### Usage

```
sensitivityProfiles(object, ...) <- value</pre>
```

# **Arguments**

object An S4 object to update the sensitivity profile summaries for.

... Fallthrough arguments for defining new methods

value An object with the new sensitivity profiles. If a matrix object is passed in, con-

verted to data.frame before assignment

### Value

Updated CoreSet

80 sensitivityRaw<-

sensitivityRaw

sensitivityRaw Generic Method

# Description

Generic function to get the raw data array for a treatment response experiment from an S4 class.

### Usage

```
sensitivityRaw(object, ...)
```

# **Arguments**

object An S4 object to extract the raw sensitivity experiment data from.
... pairlist Allow new parameters to be defined for this generic.

### Value

Depends on the implemented method

### **Examples**

```
print("Generics shouldn't need examples?")
```

sensitivityRaw<-

sensitivityRaw<- Generic

### Description

Generic function to set the raw data array for a treatment response experiment in an S4 class.

# Usage

```
sensitivityRaw(object, ...) <- value</pre>
```

# Arguments

object An S4 object to extract the raw sensitivity data from.

... pairlist Allow new parameters to be defined for this generic.

value An object containing dose and viability metrics to update the object with.

#### Value

Depends on the implemented method

```
sensitivity Slot To Long Table \\ sensitivity Slot To Long Table \ Generic
```

# **Description**

Convert the sensitivity slot in an object inheriting from a CoreSet from a list to a LongTable.

# Usage

```
sensitivitySlotToLongTable(object, ...)
```

### **Arguments**

```
object CoreSet Object inheriting from CoreSet.... Allow new arguments to be defined on this generic.
```

# Value

A LongTable object containing the data in the sensitivity slot.

# **Examples**

```
print("Generics shouldn't need examples?")
```

setOps-immutable

Subset an immutable object, returning another immutable object.

# **Description**

Subset an immutable object, returning another immutable object.

### Usage

```
subset.immutable(x, ...)
## S3 method for class 'immutable'
x[...]
## S3 method for class 'immutable'
x[[...]]
## S3 method for class 'immutable'
x$...
```

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### **Arguments**

x An R object inheriting from the "immutable" S3-class.

... Catch any additional parameters. Lets objects with arbitrary dimensions be made immutable.

# Value

An immutable subset of x.

# **Examples**

```
immut_mat <- immutable(matrix(1:100, 10, 10))
immut_mat[1:5, 1:5]</pre>
```

show,CoreSet-method

Show a CoreSet

# **Description**

Show a CoreSet

# Usage

```
## S4 method for signature 'CoreSet'
show(object)
```

# Arguments

object

CoreSet object to show via cat.

### Value

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

# See Also

cat

```
show(clevelandSmall_cSet)
```

show, LongTable-method Show method for the LongTable class

### **Description**

Show method for the LongTable class

# Usage

```
## S4 method for signature 'LongTable'
show(object)
```

### **Arguments**

object

A LongTable object to print the results for.

#### Value

invisible Prints to console.

# **Examples**

```
show(merckLongTable)
```

showSigAnnot

Get the annotations for a Signature class object, as returned by drugSensitivitysig or radSensitivtySig functions available in PharmacoGx and RadioGx, respectively.

# Description

Get the annotations for a Signature class object, as returned by drugSensitivitysig or radSensitivtySig functions available in PharmacoGx and RadioGx, respectively.

### Usage

```
showSigAnnot(object, ...)
```

# **Arguments**

object A Signature class object

... Allow definition of new arguments to this generic

# Value

NULL Prints the signature annotations to console

### **Examples**

```
print("Generics shouldn't need examples?")
```

```
subset,LongTable-method
```

Subset method for a LongTable object.

# Description

Allows use of the colData and rowData data.table objects to query based on rowID and colID, which is then used to subset all assay data.tables stored in the assays slot. This function is endomorphic, it always returns a LongTable object.

# Usage

```
## S4 method for signature 'LongTable'
subset(x, i, j, assays = assayNames(x), reindex = TRUE)
```

### **Arguments**

x	LongTable The object to subset.
i	character, numeric, logical or call Character: pass in a character vector of rownames for the LongTable object or a valid regex query which will be evaluated against the rownames. Numeric or Logical: vector of indices or a logical vector to subset the rows of a LongTable. Call: Accepts valid query statements to the data.table i parameter, this can be used to make complex queries using the data.table API for the rowData data.table.
j	character, numeric, logical or call Character: pass in a character vector of colnames for the LongTable object or a valid regex query which will be evaluated against the colnames. Numeric or Logical: vector of indices or a logical vector to subset the columns of a LongTable. Call: Accepts valid query statements to the data.table i parameter, this can be used to make complex queries using the data.table API for the colData data.table.

assays character, numeric or logical Optional list of assay names to subset. Can be used to subset the assays list further, returning only the selected items in the

new LongTable.

reindex logical(1) Should index values be reset such that they are the smallest possible

set of consecutive integers. Modifies the "rowKey", "colKey", and all assayKey columns. Initial benchmarks indicate <code>reindex=FALSE</code> saves  $\sim\!20\%$  of both execution time and memory allocation. The cost of reindexing decreases the smaller

your subset gets.

### Value

LongTable A new LongTable object subset based on the specified parameters.

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### **Examples**

summarizeMolecularProfiles

Summarize molecular profile data such that there is a single entry for each sample line/treatment combination

# Description

Summarize molecular profile data such that there is a single entry for each sample line/treatment combination

# Usage

```
summarizeMolecularProfiles(object, ...)
```

# Arguments

object An S4 object to summarize the molecular profiles for.

Allow definition of new arguments to this generic

### Value

Depends on the implemented method

```
print("Generics shouldn't need examples?")
```

summarize Sensitivity Profiles

Summarize across replicates for a sensitivity dose-response experiment

# Description

Summarize across replicates for a sensitivity dose-response experiment

# Usage

```
summarizeSensitivityProfiles(object, ...)
```

### **Arguments**

object An S4 object to summarize sensitivity profiles for.
... Allow definition of new arguments to this generic

#### Value

Depends on the implemented method

# **Examples**

```
print("Generics shouldn't need examples?")
```

TreatmentResponseExperiment

TreatmentResponseExperiment constructor method

# Description

Builds a TreatmentResponseExperiment object from rectangular objects. The rowData argument should contain row level metadata, while the colData argument should contain column level metadata, for the experimental assays in the assays list. The rowIDs and colIDs lists are used to configure the internal keys mapping rows or columns to rows in the assays. Each list should contain at minimum one character vector, specifying which columns in rowData or colData are required to uniquely identify each row. An optional second character vector can be included, specifying any metadata columns for either dimension. These should contain information about each row but NOT be required to uniquely identify a row in the colData or rowData objects. Additional metadata can be attached to a TreatmentResponseExperiment by passing a list to the metadata argument.

# Usage

```
TreatmentResponseExperiment(
  rowData,
  rowIDs,
  colData,
  colIDs,
  assays,
  assayIDs,
  metadata = list(),
  keep.rownames = FALSE
)
```

# Arguments

rowData	data.table, data.frame, matrix A table like object coercible to a data.table containing the a unique rowID column which is used to key assays, as well as additional row metadata to subset on.
rowIDs	character, integer A vector specifying the names or integer indexes of the row data identifier columns. These columns will be pasted together to make up the rownames of the TreatmentResponseExperiment object.
colData	$\label{thm:containing} \begin{tabular}{ll} $data.table$, $data.frame$, $matrix$ A table like object coercible to a $data.table$ containing the a unique colID column which is used to key assays, as well as additional column metadata to subset on. \\ \end{tabular}$
colIDs	character, integer A vector specifying the names or integer indexes of the column data identifier columns. These columns will be pasted together to make up the colnames of the TreatmentResponseExperiment object.
assays	A list containing one or more objects coercible to a data.table, and keyed by rowIDs and colIDs corresponding to the rowID and colID columns in colData and rowData.
assayIDs	list A list of character vectors specifying the columns needed to uniquely identify each row in an assay. Names must match the assays list.
metadata	A list of metadata associated with the ${\tt TreatmentResponseExperiment}$ object being constructed
keep.rownames	logical, character Logical: whether rownames should be added as a column if coercing to a data.table, default is FALSE. If TRUE, rownames are added to the column 'rn'. Character: specify a custom column name to store the rownames in.

# **Details**

For now this class is simply a wrapper around a LongTable class. In the future we plan to refactor CoreGx such that the LongTable class is in a separate pacakge. We can then specialize the implementation of TreatmentResponseExperiment to better capture the biomedical nature of this object.

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#### Value

A TreatmentResponseExperiment object containing the data for a treatment response experiment configured according to the rowIDs and coIIDs arguments.

TREDataMapper

Constructor for the TREDataMapper class, which maps from one or more raw experimental data files to the slots of a LongTable object.

### **Description**

Constructor for the TREDataMapper class, which maps from one or more raw experimental data files to the slots of a LongTable object.

# Usage

```
TREDataMapper(
  rawdata = data.frame(),
  rowDataMap = list(character(), character()),
  colDataMap = list(character(), character()),
  assayMap = list(list(character(), character())),
  metadataMap = list(character())
)
```

# Arguments

rawdata A data.frame of raw data from a treatment response experiment. This will be

coerced to a data. table internally. We recommend using joins to aggregate

your raw data if it is not present in a single file.

rowDataMap A list-like object containing two character vectors. The first is column names

in rawdata needed to uniquely identify each row, the second is additional columns which map to rows, but are not required to uniquely identify them. Rows should

be treatments.

colDataMap A list-like object containing two character vectors. The first is column names

in rawdata needed to uniquely identify each column, the second is additional columns which map to rows, but are not required to uniquely identify them.

Columns should be samples.

assayMap A list-like where each item is a list with two character vectors defining an

assay, the first containing the identifier columns in rawdata needed to uniquely identify each row an assay, and the second the rawdata columns to be mapped to that assay. The names of assayMap will be the names of the assays in the TreatmentResponseExperiment that is created when calling metaConstruct on this DataMapper object. If the character vectors have names, the value

columns will be renamed accordingly.

metadataMap A list-like where each item is a character vector of rawdata column names to

assign to the @metadata of the LongTable, where the name of that assay is the name of the list item. If names are omitted, assays will be numbered by their

index in the list.

#### **Details**

The guessMapping method can be used to test hypotheses about the cardinality of one or more sets of identifier columns. This is helpful to determine the id columns for rowDataMap and colDataMap, as well as identify columns mapping to assays or metadata.

To attach metadata not associated with rawdata, please use the metadata assignment method on your TREDataMapper. This metadata will be merge with any metadata from metadataMap and added to the LongTable which this object ultimately constructs.

### Value

A TREDataMapper object, with columns mapped to it's slots according to the various maps in the LongTableDataMapper object.

#### See Also

guessMapping

TREDataMapper-accessors

Accessing and modifying data in a TREDataMapper object.

### **Description**

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

### Usage

```
## S4 replacement method for signature 'TREDataMapper,list'
rawdata(object) <- value

## S4 method for signature 'TREDataMapper'
rowDataMap(object)

## S4 replacement method for signature 'TREDataMapper,list_OR_List'
rowDataMap(object) <- value

## S4 method for signature 'TREDataMapper'
colDataMap(object)

## S4 replacement method for signature 'TREDataMapper,list_OR_List'
colDataMap(object) <- value

## S4 method for signature 'TREDataMapper'
assayMap(object)</pre>
```

```
## S4 replacement method for signature 'TREDataMapper,list_OR_List'
assayMap(object) <- value

## S4 method for signature 'TREDataMapper'
metadataMap(object)

## S4 replacement method for signature 'TREDataMapper,list_OR_List'
metadataMap(object) <- value</pre>
```

### **Arguments**

object A TREDataMapper object to get or set data from.

value See details.

### Details

**rawdata**: Get the raw data slot from a TREDataMapper object. Returns a list-like containing one or more raw data inputs to the TREDataMapper object.

**rawdata**: Set the raw data slot from a TREDataMapper object. **value**: The list-like object to set for the rawdata slot. Note: this currently only supports data. frame or data. table objects.

**rowDataMap**: list of two character vectors, the first are the columns required to uniquely identify each row of a TREDataMapper and the second any additional row-level metadata. If the character vectors have names, the resulting columns are automatically renamed to the item name of the specified column.

**rowDataMap<-**: Update the @rowDataMap slot of a TREDataMapper object, returning an invisible NULL. Arguments:

• value: A list or List where the first item is the names of the identifier columns – columns needed to uniquely identify each row in rowData – and the second item is the metadata associated with those the identifier columns, but not required to uniquely identify rows in the object rowData.

**colDataMap**: list of two character vectors, the first are the columns required to uniquely identify each row of a TREDataMapper and the second any additional col-level metadata. If the character vectors have names, the resulting columns are automatically renamed to the item name of the specified column.

**colDataMap<-**: Update the @colDataMap slot of a TREDataMapper object, returning an invisible NULL. Arguments:

• value: A list or List where the first item is the names of the identifier columns – columns needed to uniquely identify each row in colData – and the second item is the metadata associated with those the identifier columns, but not required to uniquely identify rows in the object rowData.

**assayMap**: A list of character vectors. The name of each list item will be the assay in a LongTableDataMapper object that the columns in the character vector will be assigned to. Column renaming occurs automatically when the character vectors have names (from the value to the name).

**assayMap<-**: Updates the @assayMap slot of a TREDataMapper object, returning an invisible NULL. Arguments:

value: A list of character vectors, where the name of each list item is the name of an assay
and the values of each character vector specify the columns mapping to the assay in the S4
object the TREDataMapper constructs.

**metadataMap**: A list of character vectors. Each item is an element of the constructed objects @metadata slot.

**metadataMap<-**: Updates TREDataMapper object in-place, then returns an invisible (NULL). Arguments:

• value: A list of character vectors. The name of each list item is the name of the item in the @metadata slot of the TREDataMapper object created when metaConstruct is called on the DataMapper, and a character vector specifies the columns of @rawdata to assign to each item.

#### Value

Accessors: See details

Setters: An update TREDataMapper object, returned invisibly.

### See Also

Other DataMapper-accessors: DataMapper-accessors, LongTableDataMapper-accessors

```
rowDataMap(exampleDataMapper)
rowDataMap(exampleDataMapper) <- list(c('treatmentid'), c())
colDataMap(exampleDataMapper)
colDataMap(exampleDataMapper) <- list(c('sampleid'), c())
assayMap(exampleDataMapper)
assayMap(exampleDataMapper) <- list(sensitivity=c(viability1='viability'))
metadataMap(exampleDataMapper)
metadataMap(exampleDataMapper) <- list(object_metadata=c('metadata'))</pre>
```

TREDataMapper-class A Class for Mapping Between Raw Data and an TreatmentResponseExperiment Object

### **Description**

A Class for Mapping Between Raw Data and an TreatmentResponseExperiment Object

#### Slots

rawdata See Slots section.
rowDataMap See Slots section.
colDataMap See Slots section.
assayMap See Slots section.
metadataMap See Slots section.

### **Slots**

- rowDataMap: A list-like object containing two character vectors. The first is column names in rawdata needed to uniquely identify each row, the second is additional columns which map to rows, but are not required to uniquely identify them. Rows should be drugs.
- colDataMap: A list-like object containing two character vectors. The first is column names
  in rawdata needed to uniquely identify each column, the second is additional columns which
  map to rows, but are not required to uniquely identify them. Columns should be samples.
- assayMap A list-like where each item is a list with two elements specifying an assay, the
  first being the identifier columns in rawdata needed to uniquely identify each row an assay,
  and the second a list of rawdata columns to be mapped to that assay. The names of assayMap
  will be the names of the assays in the LongTable that is created when calling metaConstruct
  on this DataMapper object.
- metadataMap: A list-like where each item is a character vector of rawdata column names to assign to the @metadata of the LongTable, where the name of that assay is the name of the list item. If names are omitted, assays will be numbered by their index in the list.
- rawdata: A list-like object containing one or more pieces of raw data that will be processed and mapped to the slots of an S4 object.
- metadata: A List of object level metadata.

```
updateObject, CoreSet-method
```

Update the CoreSet class after changes in it struture or API

# **Description**

Update the CoreSet class after changes in it struture or API

### Usage

```
## S4 method for signature 'CoreSet'
updateObject(object, verify = FALSE, verbose = FALSE)
```

### **Arguments**

object A CoreSet object to update the class structure for.

verify A logical(1) indicating is validObject should be called after updating the

object. Defaults to TRUE, only set FALSE for debugging.

verbose TRUE or FALSE, indicating whether information about the update should be

reported

#### Value

CoreSet with update class structure.

```
updateObject,LongTable-method
```

Update the LongTable class after changes in it struture or API

### **Description**

Update the LongTable class after changes in it struture or API

### Usage

```
## S4 method for signature 'LongTable'
updateObject(object, verify = FALSE, verbose = FALSE)
```

### **Arguments**

object A LongTable object to update the class structure for.

verify A logical(1) indicating is validObject should be called after updating the

object. Defaults to TRUE, only set FALSE for debugging.

verbose TRUE or FALSE, indicating whether information about the update should be

reported

#### Value

LongTable with update class structure.

```
[,LongTable,ANY,ANY,ANY-method [LongTable Method
```

# **Description**

Single bracket subsetting for a LongTable object. See subset for more details.

### Usage

```
## S4 method for signature 'LongTable,ANY,ANY,ANY'
x[i, j, assays = assayNames(x), ..., drop = FALSE]
```

### **Arguments**

i

j

assays

X	LongTable The object to subset.
^	Long labic The object to subset.

character, numeric, logical or call Character: pass in a character vector of drug names, which will subset the object on all row id columns matching the vector. This parameter also supports valid R regex query strings which will match on the colnames of x. For convenience, \* is converted to .\* automatically. Colon can be to denote a specific part of the colnames string to query. Numeric or Logical: these select based on the rowKey from the rowData method for the LongTable. Call: Accepts valid query statements to the data. table i parameter as a call object. We have provided the function .() to conveniently convert raw R statements into a call for use in this function.

character, numeric, logical or call Character: pass in a character vector of drug names, which will subset the object on all drug id columns matching the vector. This parameter also supports regex queries. Colon can be to denote a specific part of the colnames string to query. Numeric or Logical: these select based on the rowID from the rowData method for the LongTable. Call: Accepts valid query statements to the data.table i parameter as a call object. We have provided the function .() to conveniently convert raw R statements into a call for

use in this function.

character Names of assays which should be kept in the LongTable after sub-

setting.

. . . Included to ensure drop can only be set by name.

drop logical Included for compatibility with the '[' primitive, it defaults to FALSE

and changing it does nothing.

### Details

This function is endomorphic, it always returns a LongTable object.

# Value

A LongTable containing only the data specified in the function parameters.

### **Examples**

# **Description**

Just a wrapper around assay<- for convenience. See?'assay<-,LongTable,character-method'.

# Usage

```
## S4 replacement method for signature 'LongTable, ANY, ANY' x[[i]] \leftarrow value
```

### **Arguments**

```
x A LongTable to update.i The name of the assay to update, must be in assayNames(object).value A data.frame
```

### Value

A LongTable object with the assay i updated using value.

```
merckLongTable[['sensitivity']] <- merckLongTable[['sensitivity']]</pre>
```

\$,LongTable-method

Select an assay from a LongTable object

# Description

Select an assay from a LongTable object

# Usage

```
## S4 method for signature 'LongTable'
x$name
```

# **Arguments**

x A LongTable object to retrieve an assay from name character The name of the assay to get.

### Value

```
data.frame The assay object.
```

### **Examples**

merckLongTable\$sensitivity

\$<-,LongTable-method Update an assay from a LongTable object</pre>

# Description

Update an assay from a LongTable object

# Usage

```
## S4 replacement method for signature 'LongTable'
x$name <- value</pre>
```

#### **Arguments**

x A LongTable to update an assay for.

name character(1) The name of the assay to update

value A data. frame or data. table to update the assay with.

# Value

Updates the assay name in x with value, returning an invisible NULL.

# Examples

merckLongTable\$sensitivity <- merckLongTable\$sensitivity</pre>

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