

# Package ‘PharmacoGx’

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**Type** Package

**Title** Analysis of Large-Scale Pharmacogenomic Data

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**Description** Contains a set of functions to perform large-scale analysis of pharmaco-genomic data. These include the PharmacoSet object for storing the results of pharmacogenomic experiments, as well as a number of functions for computing common summaries of drug-dose response and correlating them with the molecular features in a cancer cell-line.

**License** GPL (>= 3)

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**Collate** 'GR.R' 'GWC.R' 'PharmacoSet-class.R' 'PharmacoSet-accessors.R' 'PharmacoSet-utils.R' 'RcppExports.R' 'adaptiveMatthewCor.R' 'callingWaterfall.R' 'class-SignatureClass.R' 'computeABC.R'

```
'computeAUC.R' 'computeAUC_old.R' 'computeAmax.R'
'computeDSS.R' 'computeDrugSensitivity.R' 'computeGR.R'
'computeIC50.R' 'computeICn.R' 'computeSlope.R'
'computeSynergy.R' 'connectivityScore.R' 'cosinePerm.R'
'datasets.R' 'downloadPSet.R' 'downloadSignatures.R'
'drugDoseResponseCurve.R' 'drugPerturbationSig.R'
'filterNoisyCurves.R' 'geneDrugPerturbation.R'
'geneDrugSensitivity.R' 'geneDrugSensitivityPBCorr.R'
'geneDrugSensitivityPCorr.R' 'getRawSensitivityMatrix.R'
'globals.R' 'intersectPSets.R' 'logLogisticRegression.R'
'matthewCor.R' 'mergePSets.R' 'methods-[.R'
'methods-drugSensitivitySig.R' 'methods-intersect.R'
'methods-subsetTo.R' 'methods-summarizeMolecularProfiles.R'
'methods-summarizeSensitivityProfiles.R' 'plotPSig.R'
'rankGeneDrugPerturbation.R' 'rankGeneDrugSensitivity.R'
'sanityCheck.R' 'updateObject-methods.R' 'zzz.R'
```

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---

 .computeZIPdelta

*Vector-based version of [computeZIPdelta](#)*


---

## Description

Following the calculation of ZIP delta score as in Appendix A3. See reference for details.

## Usage

```
.computeZIPdelta(
  treatment1id,
  treatment2id,
  treatment1dose,
  treatment2dose,
  sampleid,
  HS_1,
  HS_2,
  EC50_1,
  EC50_2,
  E_inf_1,
  E_inf_2,
  combo_viability,
  ZIP = NULL,
  residual = "logcosh",
  nthread = 1L,
  show_Rsqr = FALSE
)
```

## Arguments

|                 |                                                                             |
|-----------------|-----------------------------------------------------------------------------|
| treatment1id    | character a vector of identifiers for treatment 1                           |
| treatment2id    | character a vector of identifiers for treatment 2                           |
| treatment1dose  | numeric a vector of concentrations for treatment 1                          |
| treatment2dose  | numeric a vector of concentrations for treatment 2                          |
| sampleid        | character Cell-line ID of a drug combination screening experiment.          |
| HS_1            | numeric Hill coefficient of treatment 1                                     |
| HS_2            | numeric Hill coefficient of treatment 2                                     |
| EC50_1          | numeric relative EC50 of treatment 1.                                       |
| EC50_2          | numeric relative EC50 of treatment 2.                                       |
| E_inf_1         | numeric viability produced by the maximum attainable effect of treatment 1. |
| E_inf_2         | numeric viability produced by the maximum attainable effect of treatment 2. |
| combo_viability | numeric observed viability of the two treatments combined.                  |

|                        |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |
|------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <code>ZIP</code>       | numeric pre-computed ZIP reference values. If not provided, it will be computed during delta score calculation.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |
| <code>residual</code>  | character Method used to minimise residual in fitting curves. 3 methods available: <code>c("logcosh", "normal", "Cauchy")</code> . The default method is <code>logcosh</code> . It minimises the logarithmic hyperbolic cosine loss of the residuals and provides the fastest estimation among the three methods, with fitting quality in between normal and Cauchy; recommended when fitting large-scale datasets. The other two methods minimise residuals by considering the truncated probability distribution (as in their names) for the residual. Cauchy provides the best fitting quality but also takes the longest to run. |
| <code>nthread</code>   | integer Number of cores used to perform computation. Default 1.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |
| <code>show_Rsqr</code> | logical Whether to show the 2-way curve fitting quality in the result. Default FALSE.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |

**Value**

numeric delta scores of every dose combinations for any given treatment combinations.

**References**

Yadav, B., Wennerberg, K., Aittokallio, T., & Tang, J. (2015). Searching for Drug Synergy in Complex Dose–Response Landscapes Using an Interaction Potency Model. *Computational and Structural Biotechnology Journal*, 13, 504–513. <https://doi.org/10.1016/j.csbj.2015.09.001>

**Examples**

```
## Not run:
## ZIP is optional. Will be recomputed if not provided.
combo_profiles <- CoreGx::buildComboProfiles(
  tre,
  c("HS", "EC50", "E_inf", "ZIP", "combo_viability"))
combo_profiles[,
  .computeZIPdelta(
    treatment1id = treatment1id,
    treatment2id = treatment2id,
    treatment1dose = treatment1dose,
    treatment2dose = treatment2dose,
    sampleid = sampleid,
    HS_1 = HS_1, HS_2 = HS_2,
    EC50_1 = EC50_1, EC50_2 = EC50_2,
    E_inf_1 = E_inf_1, E_inf_2 = E_inf_2,
    combo_viability = combo_viability,
    ZIP = ZIP,
    nthread = 4,
    show_Rsqr = TRUE
  )
] -> delta_scores

## End(Not run)
```

---

```
.summarizeSensProfiles
```

*Summarize the sensitivity profiles when the sensitivity slot is a LongTable*

---

## Description

Summarize the sensitivity profiles when the sensitivity slot is a LongTable

## Usage

```
.summarizeSensProfiles(
  object,
  sensitivity.measure = "auc_recomputed",
  profiles_assay = "profiles",
  treatment_col = "treatmentid",
  sample_col = "sampleid",
  cell.lines,
  drugs,
  summary.stat,
  fill.missing = TRUE
)
```

## Value

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

---

amcc

*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**

|                       |                                                                                                                                                                                                                                   |
|-----------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <code>x, y</code>     | Two paired vectors of values. Could be replicates of observations for the same experiments for example.                                                                                                                           |
| <code>step.prc</code> | 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 <code>x/y</code> . If this variable is 0, function defaults to testing all possible splits. |
| <code>min.cat</code>  | The minimum number of members per category. Classifications with less members fitting into both categories will not be considered.                                                                                                |
| <code>nperm</code>    | The number of perumation to use for estimating significance. If 0, then no p-value is calculated.                                                                                                                                 |
| <code>nthread</code>  | Number of threads to parallize over. Both the AMCC calculation and the permutation testing is done in parallel.                                                                                                                   |

**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.

**Examples**

```
amcc(0.6^(1:5), 0.5^(1:5))
```

---

|                             |                                                              |
|-----------------------------|--------------------------------------------------------------|
| <code>availablePSets</code> | <i>Return a table of PharmacoSets available for download</i> |
|-----------------------------|--------------------------------------------------------------|

---

**Description**

The function fetches a table of all PharmacoSets available for download. The table includes the dataset names, version information for the data in the PSet, the date of last update, the name of the PSet, and references for the data contained within, a DOI for the data, and a direct download link. Download can also be done using the `downloadPSet` function.

**Usage**

```
availablePSets(canonical = TRUE)
```

**Arguments**

|                        |                                                                                                                      |
|------------------------|----------------------------------------------------------------------------------------------------------------------|
| <code>canonical</code> | <code>logical(1)</code> Should available PSets show only official PSets, or should user generated PSets be included? |
|------------------------|----------------------------------------------------------------------------------------------------------------------|

**Details**

Much more information on the processing of the data and data provenance can be found at: [www.orchestra.ca](http://www.orchestra.ca)

**Value**

A data.frame with details about the available PharmacoSets objects

**Examples**

```
if (interactive()){
  availablePSets()
}
```

---

callingWaterfall

*Drug sensitivity calling using waterfall plots*

---

**Description**

1. Sensitivity calls were made using one of IC50, ActArea or Amax

**Usage**

```
callingWaterfall(
  x,
  type = c("IC50", "AUC", "AMAX"),
  intermediate.fold = c(4, 1.2, 1.2),
  cor.min.linear = 0.95,
  name = "Drug",
  plot = FALSE
)
```

**Arguments**

|                   |                                                                                                                                                                                               |
|-------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| x                 | What type of object does this take in?                                                                                                                                                        |
| type              | ic50: IC50 values in micro molar (positive values) actarea: Activity Area, that is area under the drug activity curve (positive values) amax: Activity at max concentration (positive values) |
| intermediate.fold | vector of fold changes used to define the intermediate sensitivities for ic50, actarea and amax respectively                                                                                  |
| cor.min.linear    | numeric The minimum linear correlation to require?                                                                                                                                            |
| name              | character The name of the output to use in plot                                                                                                                                               |
| plot              | boolean Whether to plot the results                                                                                                                                                           |

**Details**

1. Sort log IC50s (or ActArea or Amax) of the samples to generate a “waterfall distribution”
2. Identify cutoff:
  - 3.1 If the waterfall distribution is non-linear (pearson cc to the linear fit  $\leq 0.95$ ), estimate the major inflection point of the log IC50 curve as the point on the curve with the maximal distance to a line drawn between the start and end points of the distribution.
  - 3.2 If the waterfall distribution appears linear (pearson cc to the linear fit  $> 0.95$ ), then use the median IC50 instead.
1. Samples within a 4-fold IC50 (or within a 1.2-fold ActArea or 20% Amax difference) difference centered around this inflection point are classified as being “intermediate”, samples with lower IC50s (or ActArea/Amax values) than this range are defined as sensitive, and those with IC50s (or ActArea/Amax) higher than this range are called “insensitive”.
2. Require at least x sensitive and x insensitive samples after applying these criteria (x=5 in our case).

**Value**

factor Containing the drug sensitivity status of each sample.

**Examples**

```
# Dummy example
1 + 1
```

---

CCLEsmall

---

*Cancer Cell Line Encyclopedia (CCLE) Example PharmacoS*et

---

**Description**

A small example version of the CCLE PharmacoS

et, used in the documentation examples. All credit for the data goes to the CCLE group at the Broad Institute. This is not a full version of the dataset, most of the dataset was removed to make runnable example code. For the full dataset, please download using the downloadPSet function.**Usage**

```
data(CCLEsmall)
```

**Format**

PharmacoS

et object**References**

Barretina et al. The Cancer Cell Line Encyclopedia enables predictive modelling of anticancer drug sensitivity. Nature, 2012

---

|                    |                                                                           |
|--------------------|---------------------------------------------------------------------------|
| checkPsetStructure | <i>A function to verify the structure of a PharmacoS<small>e</small>t</i> |
|--------------------|---------------------------------------------------------------------------|

---

### Description

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

### Usage

```
checkPsetStructure(object, plotDist = FALSE, result.dir = ".")
```

### Arguments

|            |                                                                   |
|------------|-------------------------------------------------------------------|
| object     | A PharmacoS <small>e</small> t 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        |

### Value

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

### Examples

```
data(CCLEsmall)  
checkPsetStructure(CCLEsmall)
```

---

|                            |                                                            |
|----------------------------|------------------------------------------------------------|
| CMA <small>P</small> small | <i>Connectivity Map Example PharmacoS<small>e</small>t</i> |
|----------------------------|------------------------------------------------------------|

---

### Description

A small example version of the Connectivity Map PharmacoSet, used in the documentation examples. All credit for the data goes to the Connectivity Map group at the Broad Institute. This is not a full version of the dataset, most of the dataset was removed to make runnable example code. For the full dataset, please download using the downloadPSet function.

### Usage

```
data(CMAPsmall)
```

**Format**

PharmacoSet object

**References**

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

---

|            |                                                                                                      |
|------------|------------------------------------------------------------------------------------------------------|
| computeABC | <i>Fits dose-response curves to data given by the user and returns the ABC of the fitted curves.</i> |
|------------|------------------------------------------------------------------------------------------------------|

---

**Description**

Fits dose-response curves to data given by the user and returns the ABC of the fitted curves.

**Usage**

```
computeABC(
  conc1,
  conc2,
  viability1,
  viability2,
  Hill_fit1,
  Hill_fit2,
  conc_as_log = FALSE,
  viability_as_pct = TRUE,
  trunc = TRUE,
  verbose = TRUE
)
```

**Arguments**

|            |                                                                                                                                                                                                                                                                                                                                                                      |
|------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| conc1      | numeric is a vector of drug concentrations.                                                                                                                                                                                                                                                                                                                          |
| conc2      | numeric is a vector of drug concentrations.                                                                                                                                                                                                                                                                                                                          |
| viability1 | numeric is a vector whose entries are the viability values observed in the presence of the drug concentrations whose logarithms are in the corresponding entries of conc1, expressed as percentages of viability in the absence of any drug.                                                                                                                         |
| viability2 | numeric is a vector whose entries are the viability values observed in the presence of the drug concentrations whose logarithms are in the corresponding entries of conc2, expressed as percentages of viability in the absence of any drug.                                                                                                                         |
| Hill_fit1  | list or vector In the order: c("Hill Slope", "E_inf", "EC50"), the parameters of a Hill Slope as returned by logLogisticRegression. If conc_as_log is set then the function assumes logEC50 is passed in, and if viability_as_pct flag is set, it assumes E_inf is passed in as a percent. Otherwise, E_inf is assumed to be a decimal, and EC50 as a concentration. |

|                  |                                                                                                                                                                                                                                                                                                                                                                     |
|------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Hill_fit2        | lis or vector In the order: c("Hill Slope", "E_inf", "EC50"), the parameters of a Hill Slope as returned by logLogisticRegression. If conc_as_log is set then the function assumes logEC50 is passed in, and if viability_as_pct flag is set, it assumes E_inf is passed in as a percent. Otherwise, E_inf is assumed to be a decimal, and EC50 as a concentration. |
| conc_as_log      | logical, if true, assumes that log10-concentration data has been given rather than concentration data.                                                                                                                                                                                                                                                              |
| viability_as_pct | logical, if false, assumes that viability is given as a decimal rather than a percentage, and returns ABC as a decimal. Otherwise, viability is interpreted as percent, and AUC is returned 0-100.                                                                                                                                                                  |
| trunc            | logical, if true, causes viability data to be truncated to lie between 0 and 1 before curve-fitting is performed.                                                                                                                                                                                                                                                   |
| verbose          | logical, if true, causes warnings thrown by the function to be printed.                                                                                                                                                                                                                                                                                             |

**Value**

The numeric area of the absolute difference between the two hill slopes

**Author(s)**

Mark Freeman

**Examples**

```
dose1 <- c(0.0025,0.008,0.025,0.08,0.25,0.8,2.53,8)
viability1 <- c(108.67,111,102.16,100.27,90,87,74,57)
dose2 <- c(0.0025,0.008,0.025,0.08,0.25,0.8,2.53,8)
viability2 <- c(100.94,112.5,86,104.16,75,68,48,29)
computeABC(dose1, dose2, viability1, viability2)
```

---

|             |                                                                                                                                                                       |
|-------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| computeAmax | <i>Fits dose-response curves to data given by the user and returns the Amax of the fitted curve. Amax: 100 - viability at maximum concentration (in fitted curve)</i> |
|-------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------|

---

**Description**

Fits dose-response curves to data given by the user and returns the Amax of the fitted curve. Amax: 100 - viability at maximum concentration (in fitted curve)

**Usage**

```
computeAmax(concentration, viability, trunc = TRUE, verbose = FALSE)
```

**Arguments**

|               |                                                                                                                                                                                                                                                     |
|---------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| concentration | numeric is a vector of drug concentrations.                                                                                                                                                                                                         |
| viability     | numeric is a vector whose entries are the viability values observed in the presence of the drug concentrations whose logarithms are in the corresponding entries of the log_conc, expressed as percentages of viability in the absence of any drug. |
| trunc         | logical, if true, causes viability data to be truncated to lie between 0 and 1 before curve-fitting is performed.                                                                                                                                   |
| verbose       | logical should warnings be printed                                                                                                                                                                                                                  |

**Value**

The numerical Amax

**Examples**

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

---

computeAUC

---

*Computes the AUC for a Drug Dose Viability Curve*


---

**Description**

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

**Usage**

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

**Arguments**

|                  |                                                                                                                                                                                                                                                                                                                                                                      |
|------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| concentration    | numeric is a vector of drug concentrations.                                                                                                                                                                                                                                                                                                                          |
| viability        | numeric is a vector whose entries are the viability values observed in the presence of the drug concentrations whose logarithms are in the corresponding entries of conc, where viability 0 indicates that all cells died, and viability 1 indicates that the drug had no effect on the cells.                                                                       |
| Hill_fit         | list or vector In the order: c("Hill Slope", "E_inf", "EC50"), the parameters of a Hill Slope as returned by logLogisticRegression. If conc_as_log is set then the function assumes logEC50 is passed in, and if viability_as_pct flag is set, it assumes E_inf is passed in as a percent. Otherwise, E_inf is assumed to be a decimal, and EC50 as a concentration. |
| conc_as_log      | logical, if true, assumes that log10-concentration data has been given rather than concentration data.                                                                                                                                                                                                                                                               |
| viability_as_pct | logical, if false, assumes that viability is given as a decimal rather than a percentage, and returns AUC as a decimal. Otherwise, viability is interpreted as percent, and AUC is returned 0-100.                                                                                                                                                                   |
| trunc            | logical, if true, causes viability data to be truncated to lie between 0 and 1 before curve-fitting is performed.                                                                                                                                                                                                                                                    |
| area.type        | Should the area be computed using the actual data ("Actual"), or a fitted curve ("Fitted")                                                                                                                                                                                                                                                                           |
| verbose          | logical, if true, causes warnings thrown by the function to be printed.                                                                                                                                                                                                                                                                                              |

**Value**

Numeric AUC value

**Examples**

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

---

computeBliss

---

*Compute Bliss Null References*


---

**Description**

Given two numeric containing viability of two monotherapy respectively, Compute Bliss null reference values for the expected response of the two treatments combined.

**Usage**

```
computeBliss(viability_1, viability_2)
```

**Arguments**

viability\_1      numeric monotherapeutic response of treatment 1.  
viability\_2      numeric monotherapeutic response of treatment 2.

**Value**

numeric expected response of the two treatments combined under Bliss null assumption.

**Examples**

```
(bliss <- computeBliss(0.75, 0.65))
```

---

|            |                                    |
|------------|------------------------------------|
| computeHSA | <i>Compute HSA Null References</i> |
|------------|------------------------------------|

---

**Description**

Given two numeric containing viability of two monotherapy respectively, Compute highest single-agent (HSA) values as the expected response of the two treatments combined.

**Usage**

```
computeHSA(viability_1, viability_2)
```

**Arguments**

viability\_1      numeric monotherapeutic response of treatment 1.  
viability\_2      numeric monotherapeutic response of treatment 2.

**Value**

numeric expected response of the two treatments combined using the highest response of the two (lower viability).

**Examples**

```
(hsa <- computeHSA(0.75, 0.65))
```

---

computeIC50

---

*Computes the IC<sub>n</sub> for any n in 0-100 for a Drug Dose Viability Curve*


---

### Description

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

### Usage

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

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

### Arguments

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

|                  |                                                                                                                                                               |
|------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------|
| conc_as_log      | logical, if true, assumes that log10-concentration data has been given rather than concentration data, and that log10(ICn) should be returned instead of ICn. |
| viability_as_pct | logical, if false, assumes that viability is given as a decimal rather than a percentage, and that E_inf passed in as decimal.                                |
| verbose          | logical, if true, causes warnings thrown by the function to be printed.                                                                                       |
| trunc            | logical, if true, causes viability data to be truncated to lie between 0 and 1 before curve-fitting is performed.                                             |
| n                | numeric The percentile concentration to compute. If viability_as_pct set, assumed to be percentage, otherwise assumed to be a decimal value.                  |

### Value

numeric(1) The ICn of the Hill curve over the specified dose range.  
a numeric value for the concentration of the nth precentile viability reduction

### Functions

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

### Examples

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

---

|              |                                       |
|--------------|---------------------------------------|
| computeLoewe | <i>Computes Loewe Null References</i> |
|--------------|---------------------------------------|

---

### Description

Predict the response of a treatment combination under the Loewe additive null assumption.

### Usage

```
computeLoewe(
  treatment1dose,
  HS_1,
  E_inf_1,
  EC50_1,
  treatment2dose,
  HS_2,
  E_inf_2,
  EC50_2,
  tol = 0.1,
```

```

    lower_bound = 0,
    upper_bound = 1,
    verbose = FALSE
  )

```

### Arguments

|                |                                                                                                                                                 |
|----------------|-------------------------------------------------------------------------------------------------------------------------------------------------|
| treatment1dose | numeric a vector of concentrations for treatment 1                                                                                              |
| HS_1           | numeric Hill coefficient of treatment 1                                                                                                         |
| E_inf_1        | numeric viability produced by the maximum attainable effect of treatment 1.                                                                     |
| EC50_1         | numeric relative EC50 of treatment 1.                                                                                                           |
| treatment2dose | numeric a vector of concentrations for treatment 2                                                                                              |
| HS_2           | numeric Hill coefficient of treatment 2                                                                                                         |
| E_inf_2        | numeric viability produced by the maximum attainable effect of treatment 2.                                                                     |
| EC50_2         | numeric relative EC50 of treatment 2.                                                                                                           |
| tol            | numeric Error tolerance for deviations from Loewe assumption. Loewe predictions with error higher than tol will be returned as NA. Default 0.1. |
| lower_bound    | numeric Lowest possible value for Loewe expected viability. Default 0.                                                                          |
| upper_bound    | numeric Highest possible value for Loewe expected viability. Default 1.                                                                         |
| verbose        | logical whether to display warning messages. Default FALSE.                                                                                     |

### Value

numeric expected viability under Loewe additive null assumption.

### Examples

```

## Not run:
tre |>
  endoaggregate(
    assay="combo_viability",
    Loewe = computeLoewe(
      treatment1dose=treatment1dose,
      treatment2dose=treatment2dose,
      HS_1=HS_1,
      HS_2=HS_2,
      E_inf_1=E_inf_1,
      E_inf_2=E_inf_2,
      EC50_1=EC50_1,
      EC50_2=EC50_2
    ),
    by = assayKeys(tre, "combo_viability")
  ) -> tre

## End(Not run)

```

---

|              |                                                                                                                                                   |
|--------------|---------------------------------------------------------------------------------------------------------------------------------------------------|
| computeSlope | <i>Return Slope (normalized slope of the drug response curve) for an experiment of a pSet by taking its concentration and viability as input.</i> |
|--------------|---------------------------------------------------------------------------------------------------------------------------------------------------|

---

## Description

Return Slope (normalized slope of the drug response curve) for an experiment of a pSet by taking its concentration and viability as input.

## Usage

```
computeSlope(concentration, viability, trunc = TRUE, verbose = TRUE)
```

## Arguments

|               |                                                                                                                                                                                                                                           |
|---------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| concentration | numeric A concentration range that the AUC should be computed for that range. Concentration range by default considered as not logarithmic scaled. Converted to numeric by function if necessary.                                         |
| viability     | numeric Viabilities corresponding to the concentration range passed as first parameter. The range of viability values by definition should be between 0 and 100. But the viabilities greater than 100 and lower than 0 are also accepted. |
| trunc         | logical(1) A flag that identify if the viability values should be truncated to be in the range of (0,100)                                                                                                                                 |
| verbose       | logical(1) If 'TRUE' the function will retrun warnings and other infomrative messages.                                                                                                                                                    |

## Value

Returns the normalized linear slope of the drug response curve

## Examples

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

---

computeZIP

*Computes ZIP Null References*


---

### Description

Predict the additive response of a treatment combination under the ZIP null assumption.

### Usage

```
computeZIP(
  treatment1dose,
  HS_1,
  EC50_1,
  E_inf_1,
  treatment2dose,
  HS_2,
  EC50_2,
  E_inf_2
)
```

### Arguments

|                |                                                                                                              |
|----------------|--------------------------------------------------------------------------------------------------------------|
| treatment1dose | numeric a vector of concentrations for treatment 1                                                           |
| HS_1           | numeric Hill coefficient of treatment 1                                                                      |
| EC50_1         | numeric relative EC50 of treatment 1.                                                                        |
| E_inf_1        | numeric viability produced by the maximum attainable effect of treatment 1. Default 0 by the original paper. |
| treatment2dose | numeric a vector of concentrations for treatment 2                                                           |
| HS_2           | numeric Hill coefficient of treatment 2                                                                      |
| EC50_2         | numeric relative EC50 of treatment 2.                                                                        |
| E_inf_2        | numeric viability produced by maximum effect of treatment 2. Default 0 by the original paper.                |

### Value

numeric expected viability under ZIP null assumption.

### Examples

```
(zip <- computeZIP(
  treatment1dose = c(0.1, 0.01, 0.001),
  treatment2dose = c(1, 0.1, 0.01),
  HS_1 = rep(1, 3), HS_2 = rep(1.2, 3),
  EC50_1 = rep(0.01, 3), EC50_2 = rep(0.1, 3),
  E_inf_1 = rep(0, 3), E_inf_2 = rep(0.1, 3)
))
```

---

|                 |                                                              |
|-----------------|--------------------------------------------------------------|
| computeZIPdelta | <i>Generic to compute ZIP delta scores from an S4 object</i> |
|-----------------|--------------------------------------------------------------|

---

**Description**

Generic to compute ZIP delta scores from an S4 object

**Usage**

```
computeZIPdelta(object, ...)
```

**Arguments**

|        |                                            |
|--------|--------------------------------------------|
| object | S4 An object to compute delta scores from. |
| ...    | Allow new arguments to this generic.       |

**Value**

Depends on the implemented method.

**Examples**

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

---

|                                                     |
|-----------------------------------------------------|
| computeZIPdelta, TreatmentResponseExperiment-method |
| <i>Compute ZIP delta score</i>                      |

---

**Description**

Following the calculation of ZIP delta score as in Appendix A3. See reference for details.

Compute ZIP delta score as described in the original paper.

**Usage**

```
## S4 method for signature 'TreatmentResponseExperiment'
computeZIPdelta(object, residual = "logcosh", nthread = 1L, show_Rsq = FALSE)
```

**Arguments**

|          |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |
|----------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| object   | <a href="#">TreatmentResponseExperiment</a> The TreatmentResponseExperiment from which to extract assays mono_profile and combo_viability to compute ZIP delta scores.                                                                                                                                                                                                                                                                                                                                                                                                                                   |
| residual | character Method used to minimise residual in fitting curves. 3 methods available: c("logcosh", "normal", "Cauchy"). The default method is logcosh. It minimises the logarithmic hyperbolic cosine loss of the residuals and provides the fastest estimation among the three methods, with fitting quality in between normal and Cauchy; recommended when fitting large-scale datasets. The other two methods minimise residuals by considering the truncated probability distribution (as in their names) for the residual. Cauchy provides the best fitting quality but also takes the longest to run. |
| nthread  | integer Number of cores used to perform computation. Default 1.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |
| show_Rsq | logical Whether to show the 2-way curve fitting quality in the result. Default FALSE.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |

**Value**

[TreatmentResponseExperiment](#) with assay combo\_scores containing delta\_scores

**References**

Yadav, B., Wennerberg, K., Aittokallio, T., & Tang, J. (2015). Searching for Drug Synergy in Complex Dose–Response Landscapes Using an Interaction Potency Model. *Computational and Structural Biotechnology Journal*, 13, 504–513. <https://doi.org/10.1016/j.csbj.2015.09.001>

**Examples**

```
## Not run:
tre <- computeZIPdelta(tre, residual = "Cauchy", nthread = 2L)

## End(Not run)
```

---

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

**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.                                                                                   |
| y          | 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**

```
xValue <- c(1,5,23,4,8,9,2,19,11,12,13)
xSig <- c(0.01, 0.001, .97, 0.01,0.01,0.28,0.7,0.01,0.01,0.01,0.01)
yValue <- c(1,5,10,4,8,19,22,19,11,12,13)
ySig <- c(0.01, 0.001, .97,0.01, 0.01,0.78,0.9,0.01,0.01,0.01,0.01)
```

```
xx <- cbind(xValue, xSig)
yy <- cbind(yValue, ySig)
rownames(xx) <- rownames(yy) <- c('1','2','3','4','5','6','7','8','9','10','11')
data.cor <- connectivityScore(xx,yy,method='gwc', gwc.method='spearman', nperm=300)
```

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**

|                           |                                                                                                                                                                                                                                                                        |
|---------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <code>x</code>            | factor is the factors for the first variable                                                                                                                                                                                                                           |
| <code>y</code>            | factor is the factors for the second variable                                                                                                                                                                                                                          |
| <code>nperm</code>        | integer is the number of permutations to compute the null distribution of MCC estimates                                                                                                                                                                                |
| <code>alternative</code>  | 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' |
| <code>include.perm</code> | boolean indicates whether the estimates for the null distribution should be returned. Default set to 'FALSE'                                                                                                                                                           |
| <code>nthread</code>      | integer is the number of threads to be used to perform the permutations in parallel                                                                                                                                                                                    |

**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)
```

---

dim,PharmacoSet-method

*Get the dimensions of a PharmacoSet*


---

**Description**

Get the dimensions of a PharmacoSet

**Usage**

```
## S4 method for signature 'PharmacoSet'
dim(x)
```

**Arguments**

x                      PharmacoSet

**Value**

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

---

downloadPertSig

*Download Drug Perturbation Signatures*


---

**Description**

This function allows you to download an array of drug perturbation signatures, as would be computed by the drugPerturbationSig function, for the available perturbation PharmacoSets. This function allows the user to skip these very lengthy calculation steps for the datasets available, and start their analysis from the already computed signatures

**Usage**

```
downloadPertSig(
  name,
  saveDir = file.path(".", "PSets", "Sigs"),
  fileName,
  verbose = TRUE,
  ...,
  myfn
)
```

**Arguments**

|          |                                                                                                                                                                                            |
|----------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| name     | A character(1) string, the name of the PharmacoSset for which to download signatures. The name should match the names returned in the PSet Name column of availablePSets(canonical=FALSE). |
| saveDir  | A character(1) string with the folder path where the PharmacoSset should be saved. Defaults to <code>"/PSets/Sigs/"</code> . Will create directory if it does not exist.                   |
| fileName | character(1) What to name the downloaded file. Defaults to <code>'name_signature.RData'</code> when excluded.                                                                              |
| verbose  | logical(1) Should downloader show detailed messages?                                                                                                                                       |
| ...      | pairlist Force subsequent arguments to be named.                                                                                                                                           |
| myfn     | character(1) A deprecated version of fileName. Still works for now, but will be deprecated in future releases.                                                                             |

**Value**

An array type object containing the signatures

**Examples**

```
## Not run:
  if (interactive()) downloadPertSig("CMAP_2016")

## End(Not run)
```

---

|              |                                       |
|--------------|---------------------------------------|
| downloadPSet | <i>Download a PharmacoSset object</i> |
|--------------|---------------------------------------|

---

**Description**

This function allows you to download a PharmacoSset object for use with this package. The PharmacoSsets have been extensively curated and organised within a PharmacoSset class, enabling use with all the analysis tools provided in PharmacoSx. Use availablePSets to discover which PSets are available.

**Usage**

```
downloadPSet(
  name,
  saveDir = tempdir(),
  pSetFileName = NULL,
  verbose = TRUE,
  timeout = 600
)
```

**Arguments**

|              |                                                                                                                                                                       |
|--------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| name         | Character string, the name of the PharmacoSet to download. Note that this is not the dataset name, but the PSet name - dataset names are not guaranteed to be unique. |
| saveDir      | Character string with the folder path where the PharmacoSet should be saved. Defaults to <code>tempdir()</code> . Will create directory if it does not exist.         |
| pSetFileName | character string, the file name to save the dataset under                                                                                                             |
| verbose      | bool Should status messages be printed during download. Defaults to TRUE.                                                                                             |
| timeout      | numeric Parameter that lets you extend R's default timeout for downloading large files. Defaults for this function to 600.                                            |

**Value**

A PSet object with the dataset

**Warning**

BREAKING CHANGES - this function now defaults to `tempdir()` as the download path! You must specify a `saveDir` or manually save the PSet if you want your download to persist past your current R session.'

**Examples**

```
## Not run:
  if (interactive()) downloadPSet("CTRPv2_2015")

## End(Not run)
```

---

`drugDoseResponseCurve` *Plot drug response curve of a given drug and a given cell for a list of pSets (objects of the PharmacoSet class).*

---

**Description**

Given a list of PharmacoSets, the function will plot the drug\_response curve, for a given drug/cell pair. The y axis of the plot is the viability percentage and x axis is the log transformed concentrations. If more than one pSet is provided, a light gray area would show the common concentration range between pSets. User can ask for type of sensitivity measurement to be shown in the plot legend. The user can also provide a list of their own concentrations and viability values, as in the examples below, and it will be treated as experiments equivalent to values coming from a pset. The names of the concentration list determine the legend labels.

**Usage**

```

drugDoseResponseCurve(
  drug,
  cellline,
  pSets = list(),
  concentrations = list(),
  viabilities = list(),
  conc_as_log = FALSE,
  viability_as_pct = TRUE,
  trunc = TRUE,
  legends.label = c("ic50_published", "gi50_published", "auc_published",
    "auc_recomputed", "ic50_recomputed"),
  ylim = c(0, 100),
  xlim,
  mycol,
  title,
  plot.type = c("Fitted", "Actual", "Both"),
  summarize.replicates = TRUE,
  lwd = 0.5,
  cex = 0.7,
  cex.main = 0.9,
  legend.loc = "topright",
  verbose = TRUE,
  sample_col = "sampleid",
  treatment_col = "treatmentid"
)

```

**Arguments**

|                             |                                                                                                                                                                                                                    |
|-----------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| drug                        | character(1) A drug name for which the drug response curve should be plotted. If the plot is desirable for more than one pharmaco set, A unique drug id should be provided.                                        |
| cellline                    | character(1) A cell line name for which the drug response curve should be plotted. If the plot is desirable for more than one pharmaco set, A unique cell id should be provided.                                   |
| pSets                       | list a list of PharmacoSet objects, for which the function should plot the curves.                                                                                                                                 |
| concentrations, viabilities | list A list of concentrations and viabilities to plot, the function assumes that concentrations[[i]] is plotted against viabilities[[i]]. The names of the concentration list are used to create the legend labels |
| conc_as_log                 | logical, if true, assumes that log10-concentration data has been given rather than concentration data, and that log10(ICn) should be returned instead of ICn. Applies only to the concentrations parameter.        |
| viability_as_pct            | logical, if false, assumes that viability is given as a decimal rather than a percentage, and that E_inf passed in as decimal. Applies only to the viabilities parameter.                                          |

|                                   |                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
|-----------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <code>trunc</code>                | logical(1) Should the viability values be truncated to lie in [0-100] before doing the fitting                                                                                                                                                                                                                                                                                                                                                                  |
| <code>legends.label</code>        | numeric A vector of sensitivity measurment types which could be any combination of <code>ic50_published</code> , <code>auc_published</code> , <code>auc_recomputed</code> and <code>auc_recomputed_star</code> . A legend will be displayed on the top right of the plot which each line of the legend is the values of requested sensitivity measerments for one of the requested pSets. If this parameter is missed no legend would be provided for the plot. |
| <code>ylim</code>                 | numeric A vector of two numerical values to be used as ylim of the plot. If this parameter would be missed <code>c(0,100)</code> would be used as the ylim of the plot.                                                                                                                                                                                                                                                                                         |
| <code>xlim</code>                 | numeric A vector of two numerical values to be used as xlim of the plot. If this parameter would be missed the minimum and maximum comncentrations between all the pSets would be used as plot xlim.                                                                                                                                                                                                                                                            |
| <code>mycol</code>                | numeric A vector with the same lenght of the pSets parameter which will determine the color of the curve for the pharmaco sets. If this parameter is missed default colors from Rcolorbrewer package will be used as curves color.                                                                                                                                                                                                                              |
| <code>title</code>                | character The title of the graph. If no title is provided, then it defaults to 'Drug': 'Cell Line'.                                                                                                                                                                                                                                                                                                                                                             |
| <code>plot.type</code>            | character Plot type which can be the actual one ("Actual") or the one fitted by logl logistic regression ("Fitted") or both of them ("Both"). If this parameter is missed by default actual curve is plotted.                                                                                                                                                                                                                                                   |
| <code>summarize.replicates</code> | character If this parameter is set to true replicates are summarized and replicates are plotted individually otherwise                                                                                                                                                                                                                                                                                                                                          |
| <code>lwd</code>                  | numeric The line width to plot with                                                                                                                                                                                                                                                                                                                                                                                                                             |
| <code>cex</code>                  | numeric The cex parameter passed to plot                                                                                                                                                                                                                                                                                                                                                                                                                        |
| <code>cex.main</code>             | numeric The cex.main parameter passed to plot, controls the size of the titles                                                                                                                                                                                                                                                                                                                                                                                  |
| <code>legend.loc</code>           | And argument passable to <code>xy.coords</code> for the position to place the legend.                                                                                                                                                                                                                                                                                                                                                                           |
| <code>verbose</code>              | logical(1) Should warning messages about the data passed in be printed?                                                                                                                                                                                                                                                                                                                                                                                         |
| <code>sample_col</code>           | character(1) The name of the column in the profiles assay that contains the sample IDs.                                                                                                                                                                                                                                                                                                                                                                         |
| <code>treatment_col</code>        | character(1) The name of the column in the profiles assay that contains the treatment IDs.                                                                                                                                                                                                                                                                                                                                                                      |

**Value**

Plots to the active graphics device and returns an invisible NULL.

**Examples**

```
if (interactive()) {
# Manually enter the plot parameters
drugDoseResponseCurve(concentrations=list("Experiment 1"=c(.008, .04, .2, 1)),
  viabilities=list(c(100,50,30,1)), plot.type="Both")

# Generate a plot from one or more PSets
```

```
data(GDSCsmall)
drugDoseResponseCurve(drug="Doxorubicin", cellline="22RV1", pSets=GDSCsmall)
}
```

---

|                     |                                                                                                                                                               |
|---------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------|
| drugPerturbationSig | <i>Creates a signature representing gene expression (or other molecular profile) change induced by administering a drug, for use in drug effect analysis.</i> |
|---------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------|

---

## Description

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

## Usage

```
drugPerturbationSig(
  pSet,
  mDataType,
  drugs,
  cells,
  features,
  nthread = 1,
  returnValues = c("estimate", "tstat", "pvalue", "fdr"),
  verbose = FALSE
)
```

## Arguments

|           |                                                                                                                                                 |
|-----------|-------------------------------------------------------------------------------------------------------------------------------------------------|
| pSet      | <a href="#">PharmacoSet</a> a PharmacoSet of the perturbation experiment type                                                                   |
| mDataType | character which one of the molecular data types to use in the analysis, out of dna, rna, maseq, snp, cnv                                        |
| drugs     | character a vector of drug names for which to compute the signatures. Should match the names used in the PharmacoSet.                           |
| cells     | character a vector of cell names to use in computing the signatures. Should match the names used in the PharmacoSet.                            |
| features  | character a vector of features for which to compute the signatures. Should match the names used in correspondant molecular data in PharmacoSet. |
| nthread   | numeric if multiple cores are available, how many cores should the computation be parallelized over?                                            |

|              |                                                                                                          |
|--------------|----------------------------------------------------------------------------------------------------------|
| returnValues | character Which of estimate, t-stat, p-value and fdr should the function return for each gene drug pair? |
| verbose      | logical(1) Should diagnostic messages be printed? (default false)                                        |

**Value**

list a 3D array with genes in the first dimension, drugs in the second, and return values in the third.

**Examples**

```
data(CMAPsmall)
drug.perturbation <- drugPerturbationSig(CMAPsmall, mDataType="rna", nthread=1)
print(drug.perturbation)
```

---

drugSensitivitySig,PharmacoSet-method

*Creates a signature representing the association between gene expression (or other molecular profile) and drug dose response, for use in drug sensitivity analysis.*

---

**Description**

Given a PharmacoSet of the sensitivity experiment type, and a list of drugs, the function will compute a signature for the effect gene expression on the molecular profile of a cell. The function returns the estimated coefficient, the t-stat, the p-value and the false discovery rate associated with that coefficient, in a 3 dimensional array, with genes in the first direction, drugs in the second, and the selected return values in the third.

**Usage**

```
## S4 method for signature 'PharmacoSet'
drugSensitivitySig(
  object,
  mDataType,
  drugs,
  features,
  cells,
  tissues,
  sensitivity.measure = "auc_recomputed",
  molecular.summary.stat = c("mean", "median", "first", "last", "or", "and"),
  sensitivity.summary.stat = c("mean", "median", "first", "last"),
  returnValues = c("estimate", "pvalue", "fdr"),
  sensitivity.cutoff,
  standardize = c("SD", "rescale", "none"),
  molecular.cutoff = NA,
```

```

molecular.cutoff.direction = c("less", "greater"),
nthread = 1,
parallel.on = c("drug", "gene"),
modeling.method = c("anova", "pearson"),
inference.method = c("analytic", "resampling"),
verbose = TRUE,
...
)

```

## Arguments

|                                         |                                                                                                                                                                                                                                                                       |
|-----------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <code>object</code>                     | PharmacoSet a PharmacoSet of the perturbation experiment type                                                                                                                                                                                                         |
| <code>mDataType</code>                  | character which one of the molecular data types to use in the analysis, out of dna, rna, maseq, snp, cnv                                                                                                                                                              |
| <code>drugs</code>                      | character a vector of drug names for which to compute the signatures. Should match the names used in the PharmacoSet.                                                                                                                                                 |
| <code>features</code>                   | character a vector of features for which to compute the signatures. Should match the names used in correspondant molecular data in PharmacoSet.                                                                                                                       |
| <code>cells</code>                      | character allows choosing exactly which cell lines to include for the signature fitting. Should be a subset of sampleNames(pSet)                                                                                                                                      |
| <code>tissues</code>                    | character a vector of which tissue types to include in the signature fitting. Should be a subset of sampleInfo(pSet)\$tissueid                                                                                                                                        |
| <code>sensitivity.measure</code>        | character which measure of the drug dose sensitivity should the function use for its computations? Use the sensitivityMeasures function to find out what measures are available for each PSet.                                                                        |
| <code>molecular.summary.stat</code>     | character What summary statistic should be used to summarize duplicates for cell line molecular profile measurements?                                                                                                                                                 |
| <code>sensitivity.summary.stat</code>   | character What summary statistic should be used to summarize duplicates for cell line sensitivity measurements?                                                                                                                                                       |
| <code>returnValues</code>               | character Which of estimate, t-stat, p-value and fdr should the function return for each gene drug pair?                                                                                                                                                              |
| <code>sensitivity.cutoff</code>         | numeric Allows the user to binarize the sensitivity data using this threshold.                                                                                                                                                                                        |
| <code>standardize</code>                | character One of "SD", "rescale", or "none", for the form of standardization of the data to use. If "SD", the the data is scaled so that SD = 1. If rescale, then the data is scaled so that the 95% interquantile range lies in [0,1]. If none no rescaling is done. |
| <code>molecular.cutoff</code>           | Allows the user to binarize the sensitivity data using this threshold.                                                                                                                                                                                                |
| <code>molecular.cutoff.direction</code> | character One of "less" or "greater", allows to set direction of binarization.                                                                                                                                                                                        |
| <code>nthread</code>                    | numeric if multiple cores are available, how many cores should the computation be parallelized over?                                                                                                                                                                  |

|                  |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |
|------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| parallel.on      | One of "gene" or "drug", chooses which level to parallelize computation (by gene, or by drug).                                                                                                                                                                                                                                                                                                                                                                                                                         |
| modeling.method  | One of "anova" or "pearson". If "anova", nested linear models (including and excluding the molecular feature) adjusted for are fit after the data is standardized, and ANOVA is used to estimate significance. If "pearson", partial correlation adjusted for tissue of origin are fit to the data, and a Pearson t-test (or permutation) test are used. Note that the difference is in whether standardization is done across the whole dataset (anova) or within each tissue (pearson), as well as the test applied. |
| inference.method | Should "analytic" or "resampling" (permutation testing + bootstrap) inference be used to estimate significance. For permutation testing, QUICK-STOP is used to adaptively stop permutations. Resampling is currently only implemented for "pearson" modelling method.                                                                                                                                                                                                                                                  |
| verbose          | logical 'TRUE' if the warnings and other informative message should be displayed                                                                                                                                                                                                                                                                                                                                                                                                                                       |
| ...              | additional arguments not currently fully supported by the function                                                                                                                                                                                                                                                                                                                                                                                                                                                     |

**Value**

array a 3D array with genes in the first dimension, drugs in the second, and return values in the third.

**Examples**

```
data(GDSCsmall)
drug.sensitivity <- drugSensitivitySig(GDSCsmall,
  mDataType = "rna",
  nthread = 1, features = fNames(GDSCsmall, "rna")[1]
)
print(drug.sensitivity)
```

---

|              |                                          |
|--------------|------------------------------------------|
| effectToDose | <i>Inverse function of Hill equation</i> |
|--------------|------------------------------------------|

---

**Description**

For the dose-response Hill equation of a drug defined by  $E(x) = E_{inf} + \frac{1-E_{inf}}{1+(\frac{x}{EC50})^{\frac{1}{HS}}}$ , that computes the response in viability from a dose in micromole for a drug, this function is the inverse function of the Hill curve that computes the dose required to produce a given response:  $f^{-1}(E) = EC50(\frac{1-E}{E-E_{inf}})^{\frac{1}{HS}}$

**Usage**

```
effectToDose(viability, EC50, HS, E_inf, is_pct = FALSE)
```

**Arguments**

|           |                                                                                                                                    |
|-----------|------------------------------------------------------------------------------------------------------------------------------------|
| viability | numeric is a vector whose entries are the viability values in the range [0, 1] if is_pct is FALSE or [0, 100] if it is TRUE.       |
| EC50      | numeric is a vector of relative EC50 for drug-response equation.                                                                   |
| HS        | numeric Hill coefficient of the drug-response equation that represents the sigmoidity of the curve.                                |
| E_inf     | numeric the maximum attainable effect of a drug when it is administered with a infinitely high concentration.                      |
| is_pct    | logical whether both the input viability and E_inf are given in percentage ([0, 100]) rather than decimal ([0, 1]). Default FALSE. |

**Value**

numeric concentrations in micromoles required to produce viability in the corresponding entries.

**Examples**

```
dose <- effectToDose(viability = 80,
                     EC50 = 42,
                     HS = 1,
                     E_inf = 10,
                     is_pct = TRUE)
```

---

|                    |                                                                       |
|--------------------|-----------------------------------------------------------------------|
| estimateProjParams | <i>Estimate the projected Hill coefficient, efficacy, and potency</i> |
|--------------------|-----------------------------------------------------------------------|

---

**Description**

Estimate the projected shape parameter HS, efficacy E\_inf and potency EC50 in the new dose-response curve of a drug after adding another drug to it by fitting a 2-parameter dose-response curve.

**Usage**

```
estimateProjParams(
  dose_to,
  combo_viability,
  dose_add,
  EC50_add,
  HS_add,
  E_inf_add = 0,
  residual = c("logcosh", "normal", "Cauchy"),
  show_Rsqr = TRUE,
  conc_as_log = FALSE,
  optim_only = FALSE,
  loss_args = list()
)
```

**Arguments**

|                 |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
|-----------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| dose_to         | numeric a vector of concentrations of the drug being added to                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |
| combo_viability | numeric observed viability of two treatments; target for fitting curve.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         |
| dose_add        | numeric a vector of concentrations of the drug added.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |
| EC50_add        | numeric relative EC50 of the drug added.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |
| HS_add          | numeric Hill coefficient of the drug added.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |
| E_inf_add       | numeric Efficacy of the drug added.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |
| residual        | character Method used to minimise residual in fitting curves. 3 methods available: logcosh, normal, Cauchy. The default method is logcosh. It minimises the logarithmic hyperbolic cosine loss of the residuals and provides the fastest estimation among the three methods, with fitting quality in between normal and Cauchy; recommended when fitting large-scale datasets. The other two methods minimise residuals by considering the truncated probability distribution (as in their names) for the residual. Cauchy provides the best fitting quality but also takes the longest to run. |
| show_Rsqr       | logical whether to show goodness-of-fit value in the result.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |
| conc_as_log     | logical indicates whether input concentrations are in log10 scale.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |
| optim_only      | logical(1) Should the fall back methods when optim fails                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |
| loss_args       | list Additional argument to the loss function. These get passed to loss via <code>do.call</code> analogously to using <code>...</code>                                                                                                                                                                                                                                                                                                                                                                                                                                                          |

**Value**

list \* HS\_proj: Projected Hill coefficient after adding a drug \* E\_inf\_proj: Projected efficacy after adding a drug \* EC50\_proj: Projected potency after adding a drug \* E\_ninf\_proj: Projected baseline viability by the added drug \* Rsqr: if show\_Rsqr is TRUE, it will include the R squared value indicating the quality of the fit in the result.

**References**

Motulsky, H., & Christopoulos, A. (2004). Fitting dose-response curves. In Fitting models to biological data using linear and nonlinear regression: A practical guide to curve fitting. Oxford University Press.

---

|                   |                                                                                                                                                                                                                                       |
|-------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| filterNoisyCurves | <i>Viability measurements in dose-reponse curves must remain stable or decrease monotonically reflecting response to the drug being tested. filterNoisyCurves flags dose-response curves that strongly violate these assumptions.</i> |
|-------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|

---

**Description**

Viability measurements in dose-response curves must remain stable or decrease monotonically reflecting response to the drug being tested. `filterNoisyCurves` flags dose-response curves that strongly violate these assumptions.

**Usage**

```
filterNoisyCurves(
  pSet,
  epsilon = 25,
  positive.cutoff.percent = 0.8,
  mean.viability = 200,
  nthread = 1
)
```

**Arguments**

|                                      |                                                                                                                                                                                   |
|--------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <code>pSet</code>                    | <a href="#">PharmacoSet</a> a PharmacoSet object                                                                                                                                  |
| <code>epsilon</code>                 | numeric a value indicates assumed threshold for the distance between to consecutive viability values on the drug-response curve in the analysis, out of dna, rna, maseq, snp, cnv |
| <code>positive.cutoff.percent</code> | numeric This value indicates that function may violate epsilon rule for how many points on drug-response curve                                                                    |
| <code>mean.viability</code>          | numeric average expected viability value                                                                                                                                          |
| <code>nthread</code>                 | numeric if multiple cores are available, how many cores should the computation be parallelized over?                                                                              |

**Value**

a list with two elements 'noisy' containing the rownames of the noisy curves, and 'ok' containing the rownames of the non-noisy curves

**Examples**

```
data(GDSCsmall)
filterNoisyCurves(GDSCsmall)
```

---

fitTwowayZIP

---

*Two-way fitting for projected dose-response curve.*


---

**Description**

Fit projected dose-response curves with `E_min` as the viability of the treatment being added to the other treatment at a fixed dose.

**Usage**

```
fitTwowayZIP(
  combo_profiles,
  residual = "logcosh",
  show_Rsqr = TRUE,
  nthread = 1L,
  optim_only = TRUE,
  loss_args = list()
)
```

**Arguments**

|                             |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |
|-----------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <code>combo_profiles</code> | <a href="#">data.table</a> contains three parameters of dose-response curves for each single agent in a drug combination, and the observed viability of two treatments combined.                                                                                                                                                                                                                                                                                                                                                                                                                                                     |
| <code>residual</code>       | character Method used to minimise residual in fitting curves. 3 methods available: <code>c("logcosh", "normal", "Cauchy")</code> . The default method is <code>logcosh</code> . It minimises the logarithmic hyperbolic cosine loss of the residuals and provides the fastest estimation among the three methods, with fitting quality in between normal and Cauchy; recommended when fitting large-scale datasets. The other two methods minimise residuals by considering the truncated probability distribution (as in their names) for the residual. Cauchy provides the best fitting quality but also takes the longest to run. |
| <code>show_Rsqr</code>      | logical whether to show goodness-of-fit value in the result.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         |
| <code>nthread</code>        | integer Number of cores used to perform computation. Default 1.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |
| <code>optim_only</code>     | logical(1) Should the fall back methods when optim fails                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |
| <code>loss_args</code>      | list Additional argument to the loss function. These get passed to losses via <code>do.call</code> analogously to using <code>...</code>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |

**Value**

[data.table](#) contains parameters of projected dose-response curves for adding one treatment to the other.

**References**

Yadav, B., Wennerberg, K., Aittokallio, T., & Tang, J. (2015). Searching for Drug Synergy in Complex Dose–Response Landscapes Using an Interaction Potency Model. *Computational and Structural Biotechnology Journal*, 13, 504–513. <https://doi.org/10.1016/j.csbj.2015.09.001>

**Examples**

```
## Not run:
combo_profiles <- CoreGx::buildComboProfiles(tre, c("HS", "EC50", "E_inf", "viability"))
combo_twowayFit <- fitTwowayZIP(combo_profiles)

## End(Not run)
```

---

GDSCsmall

*Genomics of Drug Sensitivity in Cancer Example PharmacoS*et

---

### Description

A small example version of the Genomics of Drug Sensitivity in Cancer Project PharmacoS

et, used in the documentation examples. All credit for the data goes to the Genomics of Drug Sensitivity in Cancer Project group at the Sanger. This is not a full version of the dataset, most of the dataset was removed to make runnable example code. For the full dataset, please download using the downloadPSet function.

### Usage

```
data(GDSCsmall)
```

### Format

PharmacoS

et object

### References

Garnett et al. Systematic identification of genomic markers of drug sensitivity in cancer cells. Nature, 2012.

---

geneDrugSensitivity

*Calcualte The Gene Drug Sensitivity*


---

### Description

TODO:: Write a description!

### Usage

```
geneDrugSensitivity(
  x,
  type,
  batch,
  drugpheno,
  interaction.typeexgene = FALSE,
  model = FALSE,
  standardize = c("SD", "rescale", "none"),
  verbose = FALSE
)
```

**Arguments**

|                  |                                                                                                         |
|------------------|---------------------------------------------------------------------------------------------------------|
| x                | A numeric vector of gene expression values                                                              |
| type             | A vector of factors specifying the cell lines or type types                                             |
| batch            | A vector of factors specifying the batch                                                                |
| drugpheno        | A numeric vector of drug sensitivity values (e.g., IC50 or AUC)                                         |
| interaction.type | boolean Should interaction between gene expression and cell/type type be computed? Default set to FALSE |
| model            | boolean Should the full linear model be returned? Default set to FALSE                                  |
| standardize      | character One of 'SD', 'rescale' or 'none'                                                              |
| verbose          | boolean Should the function display messages?                                                           |

**Value**

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

**Examples**

```
print("TODO::")
```

---

```
geneDrugSensitivityPBCorr
```

*Calculate The Gene Drug Sensitivity*

---

**Description**

This version of the function uses a partial correlation instead of standardized linear models, for discrete predictive features Requires at least 3 observations per group.

**Usage**

```
geneDrugSensitivityPBCorr(
  x,
  type,
  batch,
  drugpheno,
  test = c("resampling", "analytic"),
  req_alpha = 0.05,
  nBoot = 1000,
  conf.level = 0.95,
  max_perm = getOption("PharmacoGx_Max_Perm", ceiling(1/req_alpha * 100)),
  verbose = FALSE
)
```

**Arguments**

|            |                                                                                                                                                                                                                         |
|------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| x          | A numeric vector of gene expression values                                                                                                                                                                              |
| type       | A vector of factors specifying the cell lines or type types                                                                                                                                                             |
| batch      | A vector of factors specifying the batch                                                                                                                                                                                |
| drugpheno  | A numeric vector of drug sensitivity values (e.g., IC50 or AUC)                                                                                                                                                         |
| test       | A character string indicating whether resampling or analytic based tests should be used                                                                                                                                 |
| req_alpha  | numeric, number of permutations for p value calculation                                                                                                                                                                 |
| nBoot      | numeric, number of bootstrap resamplings for confidence interval estimation                                                                                                                                             |
| conf.level | numeric, between 0 and 1. Size of the confidence interval required                                                                                                                                                      |
| max_perm   | numeric the maximum number of permutations that QUICKSTOP can do before giving up and returning NA. Can be set globally by setting the option "PharmacGx_Max_Perm", or left at the default of ceiling(1/req_alpha*100). |
| verbose    | boolean Should the function display messages?                                                                                                                                                                           |

**Value**

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

**Examples**

```
print("TODO::")
```

---

```
geneDrugSensitivityPCorr
```

*Calculate The Gene Drug Sensitivity*

---

**Description**

This version of the function uses a partial correlation instead of standardized linear models.

**Usage**

```
geneDrugSensitivityPCorr(
  x,
  type,
  batch,
  drugpheno,
  test = c("resampling", "analytic"),
  req_alpha = 0.05,
  nBoot = 1000,
  conf.level = 0.95,
  max_perm = getOption("PharmacGx_Max_Perm", ceiling(1/req_alpha * 100)),
  verbose = FALSE
)
```

**Arguments**

|                         |                                                                                                                                                                                                                                       |
|-------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <code>x</code>          | A numeric vector of gene expression values                                                                                                                                                                                            |
| <code>type</code>       | A vector of factors specifying the cell lines or type types                                                                                                                                                                           |
| <code>batch</code>      | A vector of factors specifying the batch                                                                                                                                                                                              |
| <code>drugpheno</code>  | A numeric vector of drug sensitivity values (e.g., IC50 or AUC)                                                                                                                                                                       |
| <code>test</code>       | A character string indicating whether resampling or analytic based tests should be used                                                                                                                                               |
| <code>req_alpha</code>  | numeric, number of permutations for p value calculation                                                                                                                                                                               |
| <code>nBoot</code>      | numeric, number of bootstrap resamplings for confidence interval estimation                                                                                                                                                           |
| <code>conf.level</code> | numeric, between 0 and 1. Size of the confidence interval required                                                                                                                                                                    |
| <code>max_perm</code>   | numeric the maximum number of permutations that QUICKSTOP can do before giving up and returning NA. Can be set globally by setting the option "PharmacGx_Max_Perm", or left at the default of <code>ceiling(1/req_alpha*100)</code> . |
| <code>verbose</code>    | boolean Should the function display messages?                                                                                                                                                                                         |

**Value**

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

**Examples**

```
print("TODO::")
```

---

|                  |                  |
|------------------|------------------|
| <code>gwc</code> | <i>GWC Score</i> |
|------------------|------------------|

---

**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 statistics) 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 statistics) for the second experiment           |
| p2         | numeric vector of p-values for each corresponding effect size for the second experiment     |
| 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(CCLEsmall)
x <- molecularProfiles(CCLEsmall,"rna")[,1]
y <- molecularProfiles(CCLEsmall,"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)
```

---

HDAC\_genes

*HDAC Gene Signature*


---

**Description**

A gene signature for HDAC inhibitors, as detailed by Glaser et al. The signature is mapped from the probe to gene level using probeGeneMapping

**Usage**

```
data(HDAC_genes)
```

**Format**

a 13x2 data.frame with gene identifiers in the first column and direction change in the second

## References

Glaser et al. Gene expression profiling of multiple histone deacetylase (HDAC) inhibitors: defining a common gene set produced by HDAC inhibition in T24 and MDA carcinoma cell lines. Molecular cancer therapeutics, 2003.

---

hillCurve

---

4-Parameter Hill Equation for Stimuli-Response Curves

---

## Description

Sigmoidal function which fits well to many stimuli-response associations observed in biology and pharmacology. In the context of PharmacGx we are using it to model treatment-response associations in cancer cell lines.

## Usage

```
hillCurve(dose, HS, EC50, E_inf, E_ninf)
```

## Arguments

|        |                                                                                                                                                                                                                                                                                 |
|--------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| dose   | numeric() A vector of $\log_{10}(\text{dose})$ values (or equivalent for the stimuli being modelled).                                                                                                                                                                           |
| HS     | numeric(1) Hill coefficient (n) which defines the slope of the dose-response curve at the mid-point. This parameter describes the degree of sigmoidicity of the Hill curve. HS = 1 corresponds to the rectangular hyperbola in dose-response space.                             |
| EC50   | numeric(1) The dose required to produce 50% of the theoretically maximal response in the system, E_inf. Should be in the same units as dose!                                                                                                                                    |
| E_inf  | numeric(1) Theoretical maximal response (minimal viability) in the system as a proportion in the range $[0, 1]$ . Note that since we are predicting viability (percent of cells alive after treatment) instead of response, this value should be low (i.e., more cell killing). |
| E_ninf | numeric(1) Theoretical minimum response (basal response). Defaults to 1, which should be the case for most viability experiments since we expect no cell killing to occur prior to applying a treatment.                                                                        |

## Value

numeric() Vector of predicted viabilities for the Hill curve defined by EC50, E\_inf, E\_ninf and HS for each supplied value of dose.

## Author(s)

Feifei Li Petr Smirnov Christopher Eeles

## References

Gesztelyi, R., Zsuga, J., Kemeny-Beke, A., Varga, B., Juhasz, B., & Tosaki, A. (2012). The Hill equation and the origin of quantitative pharmacology. *Archive for History of Exact Sciences*, 66(4), 427–438. <https://doi.org/10.1007/s00407-012-0098-5>

Motulsky, H., & Christopoulos, A. (2004). *Fitting models to biological data using linear and non-linear regression: A practical guide to curve fitting*. Oxford University Press. See Chapter 41.

## Examples

```
(viability <- hillCurve(
  dose=c(0.1, 0.01, 0.001),
  HS=1.1,
  EC50=0.01,
  E_ninf=1,
  E_inf=0
))
```

---

|               |                                                                                                                                    |
|---------------|------------------------------------------------------------------------------------------------------------------------------------|
| intersectPSet | <i>Intersects objects of the PharmacoSet class, subsetting them to the common drugs and/or cell lines as selected by the user.</i> |
|---------------|------------------------------------------------------------------------------------------------------------------------------------|

---

## Description

Given a list of PharmacoSets, the function will find the common drugs, and/or cell lines, and return PharmacoSets that contain data only pertaining to the common drugs, and/or cell lines. The mapping between dataset drug and cell names is done using annotations found in the PharmacoSet object's internal curation slot

## Usage

```
intersectPSet(
  pSets,
  intersectOn = c("drugs", "cell.lines", "concentrations"),
  cells,
  drugs,
  strictIntersect = FALSE,
  verbose = TRUE,
  nthread = 1
)
```

## Arguments

|             |                                                                                        |
|-------------|----------------------------------------------------------------------------------------|
| pSets       | list a list of PharmacoSet objects, of which the function should find the intersection |
| intersectOn | character which identifiers to intersect on, drugs, cell lines, or concentrations      |

|                 |                                                                                                                                                                           |
|-----------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| cells           | a character vector of common cell lines between pSets. In case user is intersted on getting intersection on certain cell lines, they can provide their list of cell lines |
| drugs           | a character vector of common drugs between pSets. In case user is intersted on getting intersection on certain drugs, they can provide their list of drugs.               |
| strictIntersect | boolean Should the intersection keep only the drugs and cell lines that have been tested on together?                                                                     |
| verbose         | boolean Should the function announce its key steps?                                                                                                                       |
| nthread         | numeric The number of cores to use to run intersection on concentrations                                                                                                  |

Value

A list of pSets, contatining only the intersection

Examples

```
data(GDSCsmall)
data(CCLEsmall)
common <- intersectPSet(list('GDSC'=GDSCsmall,'CCLE'=CCLEsmall),
                        intersectOn = c("drugs", "cell.lines"))

common$CGP
common$CCLE
```

---

|         |                                              |
|---------|----------------------------------------------|
| loeweCI | <i>Loewe Additive Combination Index (CI)</i> |
|---------|----------------------------------------------|

---

Description

Computes the Loewe additive combination index (CI) from its definition  $CI = \frac{x_1}{f_1^{-1}(E)} + \frac{x_2}{f_2^{-1}(E)}$

Usage

```
loeweCI(
  viability,
  treatment1dose,
  HS_1,
  E_inf_1,
  EC50_1,
  treatment2dose,
  HS_2,
  E_inf_2,
  EC50_2,
  is_pct = FALSE
)
```

**Arguments**

|                |                                                                                                                                    |
|----------------|------------------------------------------------------------------------------------------------------------------------------------|
| viability      | numeric is a vector whose entries are the viability values in the range [0, 1].                                                    |
| treatment1dose | numeric a vector of concentrations for treatment 1                                                                                 |
| HS_1           | numeric Hill coefficient of treatment 1                                                                                            |
| E_inf_1        | numeric the maximum attainable effect of treatment 1.                                                                              |
| EC50_1         | numeric relative EC50 of treatment 1.                                                                                              |
| treatment2dose | numeric a vector of concentrations for treatment 2                                                                                 |
| HS_2           | numeric Hill coefficient of treatment 2                                                                                            |
| E_inf_2        | numeric the maximum attainable effect of treatment 2.                                                                              |
| EC50_2         | numeric relative EC50 of treatment 2.                                                                                              |
| is_pct         | logical whether both the input viability and E_inf are given in percentage ([0, 100]) rather than decimal ([0, 1]). Default FALSE. |

**Value**

CI under Loewe additive definition

**Examples**

```
## Not run:
tre |>
  endoaggregate(
    assay="combo_viability",
    Loewe = PharmacGx::computeLoewe(
      treatment1dose = treatment1dose,
      treatment2dose = treatment2dose,
      HS_1 = HS_1,
      HS_2 = HS_2,
      E_inf_1 = E_inf_1,
      E_inf_2 = E_inf_2,
      EC50_1 = EC50_1,
      EC50_2 = EC50_2
    ),
    by = assayKeys(tre, "combo_viability")
  ) -> tre

## End(Not run)
```

---

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

---

## Description

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

## Usage

```
logLogisticRegression(
  conc,
  viability,
  density = c(2, 10, 5),
  step = 0.5/density,
  precision = 1e-04,
  lower_bounds = c(0, 0, -6),
  upper_bounds = c(4, 1, 6),
  scale = 0.07,
  family = c("normal", "Cauchy"),
  median_n = 1,
  conc_as_log = FALSE,
  viability_as_pct = TRUE,
  trunc = TRUE,
  verbose = TRUE
)
```

## Arguments

|              |                                                                                                                                                                                                                                                                                                                     |
|--------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| conc         | numeric is a vector of drug concentrations.                                                                                                                                                                                                                                                                         |
| viability    | numeric is a vector whose entries are the viability values observed in the presence of the drug concentrations whose logarithms are in the corresponding entries of the log_conc, where viability 0 indicates that all cells died, and viability 1 indicates that the drug had no effect on the cells.              |
| density      | numeric is a vector of length 3 whose components are the numbers of lattice points per unit length along the HS-, E_inf-, and base-10 logarithm of the EC50-dimensions of the parameter space, respectively.                                                                                                        |
| step         | numeric is a vector of length 3 whose entries are the initial step sizes in the HS, E_inf, and base-10 logarithm of the EC50 dimensions, respectively, for the PatternSearch algorithm.                                                                                                                             |
| precision    | is a positive real number such that when the ratio of current step size to initial step size falls below it, the PatternSearch algorithm terminates. A smaller value will cause LogisticPatternSearch to take longer to complete optimization, but will produce a more accurate estimate for the fitted parameters. |
| lower_bounds | numeric is a vector of length 3 whose entries are the lower bounds on the HS, E_inf, and base-10 logarithm of the EC50 parameters, respectively.                                                                                                                                                                    |
| upper_bounds | numeric is a vector of length 3 whose entries are the upper bounds on the HS, E_inf, and base-10 logarithm of the EC50 parameters, respectively.                                                                                                                                                                    |

|                  |                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |
|------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| scale            | is a positive real number specifying the shape parameter of the Cauchy distribution.                                                                                                                                                                                                                                                                                                                                                                                   |
| family           | character, if "cauchy", uses MLE under an assumption of Cauchy-distributed errors instead of sum-of-squared-residuals as the objective function for assessing goodness-of-fit of dose-response curves to the data. Otherwise, if "normal", uses MLE with a gaussian assumption of errors                                                                                                                                                                               |
| median_n         | If the viability points being fit were medians of measurements, they are expected to follow a median of family distribution, which is in general quite different from the case of one measurement. Median_n is the number of measurements the median was taken of. If the measurements are means of values, then both the Normal and the Cauchy distributions are stable, so means of Cauchy or Normal distributed variables are still Cauchy and normal respectively. |
| conc_as_log      | logical, if true, assumes that log10-concentration data has been given rather than concentration data, and that log10(EC50) should be returned instead of EC50.                                                                                                                                                                                                                                                                                                        |
| viability_as_pct | logical, if false, assumes that viability is given as a decimal rather than a percentage, and that E_inf should be returned as a decimal rather than a percentage.                                                                                                                                                                                                                                                                                                     |
| trunc            | logical, if true, causes viability data to be truncated to lie between 0 and 1 before curve-fitting is performed.                                                                                                                                                                                                                                                                                                                                                      |
| verbose          | logical, if true, causes warnings thrown by the function to be printed.                                                                                                                                                                                                                                                                                                                                                                                                |

### Value

A list containing estimates for HS, E\_inf, and EC50. It is annotated with the attribute Rsquared, which is the  $R^2$  of the fit. Note that this is calculated using the values actually used for the fit, after truncation and any transform applied. With truncation, this will be different from the  $R^2$  compared to the variance of the raw data. This also means that if all points were truncated down or up, there is no variance in the data, and the  $R^2$  may be NaN.

### Examples

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

---

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)
```

**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 permutation testing is done |
| nthread | numeric can parallelize permutation testing using BiocParallels bplapply                         |

**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.

**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)
```

---

|                     |                                                               |
|---------------------|---------------------------------------------------------------|
| partialCorQUICKSTOP | <i>QUICKSTOP significance testing for partial correlation</i> |
|---------------------|---------------------------------------------------------------|

---

**Description**

This function will test whether the observed partial correlation is significant at a level of `req_alpha`, doing up to `MaxIter` permutations. Currently, it supports only grouping by discrete categories when calculating a partial correlation. Currently, only does two sided tests.

**Usage**

```
partialCorQUICKSTOP(
  pin_x,
  pin_y,
  pobsCor,
  pGroupFactor,
  pGroupSize,
  pnumGroup,
  pMaxIter,
  pn,
  preq_alpha,
```

```

    ptolerance_par,
    plog_decision_boundary,
    pseed
  )

```

### Arguments

|                                     |                                                                                                                                                                                                                                            |
|-------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <code>pin_x</code>                  | one of the two vectors to correlate.                                                                                                                                                                                                       |
| <code>pin_y</code>                  | the other vector to calculate                                                                                                                                                                                                              |
| <code>pobsCor</code>                | the observed (partial) correlation between these variables                                                                                                                                                                                 |
| <code>pGroupFactor</code>           | an integer vector labeling group membership, to correct for in the partial correlation. NEEDS TO BE ZERO BASED!                                                                                                                            |
| <code>pGroupSize</code>             | an integer vector of size <code>length(unique(pGroupFactor))</code> , counting the number of members of each group (basically <code>table(pGroupFactor)</code> ) as integer vector                                                         |
| <code>pnumGroup</code>              | how many groups are there ( <code>len(pGroupSize)</code> )                                                                                                                                                                                 |
| <code>pMaxIter</code>               | maximum number of iterations to do, as a REAL NUMBER                                                                                                                                                                                       |
| <code>pn</code>                     | length of x and y, as a REAL NUMBER                                                                                                                                                                                                        |
| <code>preq_alpha</code>             | the required alpha for significance                                                                                                                                                                                                        |
| <code>ptolerance_par</code>         | the tolerance region for quickstop. Suggested to be 1/100th of <code>req_alpha</code>                                                                                                                                                      |
| <code>plog_decision_boundary</code> | $\log(\text{base } e)$ of 1/probability of incorrectly calling significance, as per quickstop paper (used to determine the log-odds)                                                                                                       |
| <code>pseed</code>                  | A numeric vector of length 2, used to seed the internal xoroshiro128+ 1.0 random number generator. Note that currently, these values get modified per call, so pass in a copy if you wish to keep a seed for running same simulation twice |

### Value

a double vector of length 4, entry 1 is either 0, 1 (for TRUE/FALSE) or `NA_REAL` for significance determination `NA_REAL` is returned when the `MaxIter` were reached before a decision is made. Usually, this occurs when the real p value is close to, or falls within the tolerance region of (`req_alpha`, `req_alpha+tolerance_par`). Entry 2 is the current p value estimate. entry 3 is the total number of iterations performed. Entry 4 is the number of time a permuted value was larger in absolute value than the observed cor.

---

PharmacoSet

*PharmacoSet* constructor

---

### Description

A constructor that simplifies the process of creating `PharmacoSets`, 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 `PharmacoSet` methods. For a much more detailed instruction on creating `PharmacoSets`, please see the "CreatingPharmacoSet" vignette.

**Usage**

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

**Arguments**

|                                                   |                                                                                                                                                                                                                                                                                     |
|---------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| name                                              | A character string detailing the name of the dataset                                                                                                                                                                                                                                |
| molecularProfiles                                 | A list of SummarizedExperiment objects containing molecular profiles for each molecular data type.                                                                                                                                                                                  |
| sample                                            | A data.frame containing the annotations for all the sample profiled in the data set, across all data types. Must contain the mandatory sampleid column which uniquely identifies each sample in the object.                                                                         |
| treatment                                         | A data.frame containing annotations for all treatments profiled in the dataset. Must contain the mandatory treatmentid column which uniquely identifies each treatment in the object.                                                                                               |
| sensitivityInfo                                   | A data.frame containing the information for the sensitivity experiments. Must contain a 'sampleid' column with unique identifiers to each sample, matching the sample object and a 'treatmentid' columns with unique identifiers for each treatment, matching the treatment object. |
| sensitivityRaw                                    | A 3 Dimensional array containing the raw drug dose response data for the sensitivity experiments                                                                                                                                                                                    |
| sensitivityProfiles                               | data.frame containing drug sensitivity profile statistics such as IC50 and AUC                                                                                                                                                                                                      |
| sensitivityN, perturbationN                       | A data.frame summarizing the available sensitivity/perturbation data                                                                                                                                                                                                                |
| curationSample, curationTissue, curationTreatment | A data.frame mapping the names for samples, tissues and treatments used in the data set to universal identifiers used between different CoreSet objects                                                                                                                             |

|             |                                                                                                                                                              |
|-------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------|
| datasetType | A character(1) string of 'sensitivity', '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.                                                                                                           |

**Value**

An object of class PharmacoSet

**Examples**

```
## For help creating a PharmacoSet object, please see the following vignette:
browseVignettes("PharmacoGx")
```

---

PharmacoSet-accessors *Accessing and modifying information in a PharmacoSet*

---

**Description**

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

**Usage**

```
drugInfo(...)

drugInfo(...) <- value

drugNames(...)

drugNames(...) <- value

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

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

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

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

## S4 method for signature 'PharmacoSet'
```

```
name(object)

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

## S4 method for signature 'PharmacoSet,character'
```

```
fNames(object, mDataType)

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

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

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

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

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

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

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

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

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

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

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

## S4 method for signature 'PharmacoSet'
sensitivityRaw(object)

## S4 replacement method for signature 'PharmacoSet,array'
sensitivityRaw(object) <- value

## S4 method for signature 'PharmacoSet'
treatmentResponse(object)

## S4 replacement method for signature 'PharmacoSet,list_OR_LongTable'
treatmentResponse(object) <- value

## S4 method for signature 'PharmacoSet'
```

```

sensNumber(object)

## S4 replacement method for signature 'PharmacoSet,matrix'
sensNumber(object) <- value

## S4 method for signature 'PharmacoSet'
pertNumber(object)

## S4 replacement method for signature 'PharmacoSet,array'
pertNumber(object) <- value

```

### Arguments

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

### Details

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

- object: PharmacoSet An object to retrieve treatment metadata from.

**treatmentInfo<-:** PharmacoSet object with updated treatment metadata. object. Arguments:

- object: PharmacoSet 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 PharmacoSet object. Arguments:

- object: PharmacoSet An object to retrieve treatment names from.

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

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

#### @annotation:

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

**@dateCreated:**

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

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

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

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

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

- value: character(1) The name of the PharmacoSet object.

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

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

- value: a data.frame object.

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

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

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

**@curation:**

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

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

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

**datasetType slot:**

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

**datasetType<-:** Update the datasetType slot of a PharmacoSet 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 PharmacoSet 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 PharmacoSet 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 PharmacoSet 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 PharmacoSet 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 PharmacoSet object. More specifically, retrieve the @rowData slot from the SummarizedExperiment from the @molecularProfiles of a PharmacoSet 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 PharmacoSet object.

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

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

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

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

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

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

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

**molecularProfilesSlot<-:** Update the contents of the `@molecularProfiles` slot of a `PharmacoSet` object. Arguments:

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

#### **@treatmentResponse:**

##### *Arguments::*

- dimension: Optional character(1) One of 'treatment', 'sample' or 'assay' to retrieve `rowData`, `colData` or the 'assay\_metadata' assay from the `PharmacoSet` `@sensitivity` `LongTable` object, respectively. Ignored with warning if `@treatmentResponse` is not a `LongTable` object.
- ...: Additional arguments to the `rowData` or `colData`. `LongTable` methods. Only used if the sensitivity slot contains a `LongTable` object instead of a list and the dimension argument is specified.

##### *Methods::*

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

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

- value: A `data.frame` of treatment response experiment metadata, documenting experiment level metadata (mapping to treatments and samples). If the `@treatmentResponse` slot doesn't contain a `LongTable` and dimension is not specified, you can only modify existing columns as returned by `sensitivityInfo(object)`.

**sensitivityMeasures:** Get the 'sensitivityMeasures' available in a `PharmacoSet` object. Each measure represents some summary of sample sensitivity to a given treatment, such as `ic50`, `ec50`, `AUC`, `AAC`, etc. The results are returned as a character vector with all available metrics for the `PSet` object.

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

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

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

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

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

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

- 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 PharmacSet 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 PharmacSet object. Will error when @sensitivity contains a LongTable object, since the counts are computed on the fly. Arguments:

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

**pertNumber:** array Summary of available perturbation experiments from in a PharmacSet 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 PharmacSet 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 PharmacSet object, returned invisibly.

## Examples

```
data(CCLEsmall)
treatmentInfo(CCLEsmall)

treatmentInfo(CCLEsmall) <- treatmentInfo(CCLEsmall)

treatmentNames(CCLEsmall)

treatmentNames(CCLEsmall) <- treatmentNames(CCLEsmall)
```

```
## @annotation

annotation(CCLEsmall)

annotation(CCLEsmall) <- annotation(CCLEsmall)

dateCreated(CCLEsmall)

## dateCreated
dateCreated(CCLEsmall) <- date()

name(CCLEsmall)

name(CCLEsmall) <- 'new_name'

sampleInfo(CCLEsmall) <- sampleInfo(CCLEsmall)

sampleNames(CCLEsmall)

sampleNames(CCLEsmall) <- sampleNames(CCLEsmall)

## curation
curation(CCLEsmall)

curation(CCLEsmall) <- curation(CCLEsmall)

datasetType(CCLEsmall)

datasetType(CCLEsmall) <- 'both'

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

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

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

featureInfo(CCLEsmall, 'rna')

featureInfo(CCLEsmall, 'rna') <- featureInfo(CCLEsmall, 'rna')

phenoInfo(CCLEsmall, 'rna')

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

fNames(CCLEsmall, 'rna')

fNames(CCLEsmall, 'rna') <- fNames(CCLEsmall, 'rna')
```

```

mDataNames(CCLEsmall)

mDataNames(CCLEsmall) <- mDataNames(CCLEsmall)

molecularProfilesSlot(CCLEsmall)

molecularProfilesSlot(CCLEsmall) <- molecularProfilesSlot(CCLEsmall)

sensitivityInfo(CCLEsmall)

sensitivityInfo(CCLEsmall) <- sensitivityInfo(CCLEsmall)

sensitivityMeasures(CCLEsmall) <- sensitivityMeasures(CCLEsmall)

sensitivityMeasures(CCLEsmall) <- sensitivityMeasures(CCLEsmall)

sensitivityProfiles(CCLEsmall)

sensitivityProfiles(CCLEsmall) <- sensitivityProfiles(CCLEsmall)

head(sensitivityRaw(CCLEsmall))

sensitivityRaw(CCLEsmall) <- sensitivityRaw(CCLEsmall)

treatmentResponse(CCLEsmall)

treatmentResponse(CCLEsmall) <- treatmentResponse(CCLEsmall)

sensNumber(CCLEsmall)

sensNumber(CCLEsmall) <- sensNumber(CCLEsmall)

pertNumber(CCLEsmall)

pertNumber(CCLEsmall) <- pertNumber(CCLEsmall)

```

---

|                   |                                                                                  |
|-------------------|----------------------------------------------------------------------------------|
| PharmacoSet-class | <i>A Class to Contain PharmacoGenomic datasets together with their curations</i> |
|-------------------|----------------------------------------------------------------------------------|

---

## Description

The PharmacoSet (pSet) class was developed to contain and organise large PharmacoGenomic datasets, and aid in their metanalysis. It was designed primarily to allow bioinformaticians and biologists to work with data at the level of genes, drugs and cell lines, providing a more naturally intuitive interface and simplifying analyses between several datasets. As such, it was designed to be flexible enough to hold datasets of two different natures while providing a common interface. The

class can accomodate datasets containing both drug dose response data, as well as datasets containing genetic profiles of cell lines pre and post treatment with compounds, known respectively as sensitivity and perturbation datasets.

### Arguments

|           |                                                              |
|-----------|--------------------------------------------------------------|
| object    | A PharmacoSet object                                         |
| mDataType | A character with the type of molecular data to return/update |
| value     | A replacement value                                          |

### Value

An object of the PharmacoSet class

### Slots

|                   |                                                                                                                                                                                                                                                                                                                              |
|-------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| annotation        | A list of annotation data about the PharmacoSet, including the \$name and the session information for how the object was creating, detailing the exact versions of R and all the packages used                                                                                                                               |
| molecularProfiles | A list containing SummarizedExperiment type object for holding data for RNA, DNA, SNP and CNV measurements, with associated fData and pData containing the row and column metadata                                                                                                                                           |
| sample            | A data.frame containing the annotations for all the cell lines profiled in the data set, across all data types                                                                                                                                                                                                               |
| treatment         | A data.frame containg the annotations for all the drugs profiled in the data set, across all data types                                                                                                                                                                                                                      |
| treatmentResponse | A list containing all the data for the sensitivity experiments, including \$info, a data.frame containing the experimental info,\$raw a 3D array containing raw data, \$profiles, a data.frame containing sensitivity profiles statistics, and \$n, a data.frame detailing the number of experiments for each cell-drug pair |
| perturbation      | A list containing \$n, a data.frame summarizing the available perturbation data,                                                                                                                                                                                                                                             |
| curation          | A list containing mappings for \$treatment, cell, tissue names used in the data set to universal identifiers used between different PharmacoSet objects                                                                                                                                                                      |
| datasetType       | A character string of 'sensitivity', 'perturbation', or both detailing what type of data can be found in the PharmacoSet, for proper processing of the data                                                                                                                                                                  |

---

PharmacoSet-utils

*Utility methods for a PharmacoSet object.*


---

### Description

Documentation for utility methods for a PharmacoSet 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 'PharmacoSet'  
subsetBySample(x, samples)
```

```
## S4 method for signature 'PharmacoSet'  
subsetByTreatment(x, treatments)
```

```
## S4 method for signature 'PharmacoSet'  
subsetByFeature(x, features, mDataTypes)
```

## Arguments

|            |                                                                                                                                                 |
|------------|-------------------------------------------------------------------------------------------------------------------------------------------------|
| x          | A PharmacoSet 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 PharmacoSet object by sample identifier.

- value: a PharmacoSet object containing only samples.

### subset methods:

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

- value: a PharmacoSet object containing only treatments.

### subset methods:

**subsetByFeature:** Subset a PharmacoSet object by molecular feature identifier.

- value: a PharmacoSet object containing only features.

## Value

See details.

## Examples

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

```

CCLEsmall_sub <- subsetBySample(CCLEsmall, samples)

## subset methods

### subsetByTreatment
#treatments <- drugInfo(CCLEsmall)$drugid[seq_len(10)]
#CCLEsmall_sub <- subsetByTreatment(CCLEsmall, treatments)

## subset methods

### subsetByFeature
features <- fName(CCLEsmall, 'rna')[seq_len(5)]
CCLEsmall_sub <- subsetByFeature(CCLEsmall, features, 'rna')

```

---

PharmacoSet2

---

*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

```

PharmacoSet2(
  name = "emptySet",
  treatment = data.frame(),
  sample = data.frame(),
  molecularProfiles = MultiAssayExperiment(),
  treatmentResponse = TreatmentResponseExperiment(),
  perturbation = list(),
  curation = list(sample = data.frame(), treatment = data.frame(), tissue = data.frame()),
  datasetType = "sensitivity"
)

```

## Arguments

|           |                                                                                                                                                                    |
|-----------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| name      | A character(1) vector with the PharmacoSet objects name.                                                                                                           |
| treatment | A data.frame with treatment level metadata. Treatments in a PharmacoSet represent pharmaceutical compounds.                                                        |
| sample    | A data.frame with sample level metadata for the union of samples in treatmentResponse and molecularProfiles. Samples in a PharmacoSet represent cancer cell-lines. |

|                   |                                                                                                                          |
|-------------------|--------------------------------------------------------------------------------------------------------------------------|
| molecularProfiles | A MultiAssayExperiment containing one SummarizedExperiment object for each molecular data type.                          |
| treatmentResponse | A LongTable or LongTableDataMapper object containing all treatment response data associated with the PharmacoSig object. |
| perturbation      | A deprecated slot in a PharmacoSig object included for backwards compatibility. This may be removed in future releases.  |
| curation          | This class requires an additional curation item, tissue, which maps from published to standardized tissue identifiers.   |
| datasetType       | A deprecated slot in a PharmacoSig object included for backwards compatibility. This may be removed in future releases.  |

## Value

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

## Examples

```
data(CCLEsmall)
CCLEsmall
```

---

PharmacoSig

---

*Constructor for the PharmacoSig S4 class*


---

## Description

Constructor for the PharmacoSig S4 class

## Usage

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

**Arguments**

|             |                                                                                                             |
|-------------|-------------------------------------------------------------------------------------------------------------|
| Data        | of data to build the signature from                                                                         |
| PSetName    | character vector containing name of PSet, defaults to ""                                                    |
| DateCreated | date date the signature was created, defaults to date()                                                     |
| SigType     | character vector specifying whether the signature is sensitivity or perturbation, defaults to 'sensitivity' |
| SessionInfo | sessionInfo object as returned by sessionInfo() function, defaults to sessionInfo()                         |
| Call        | character or call specifying the constructor call used to make the object, defaults to 'No Call Recorded'   |
| Arguments   | list a list of additional arguments to the constructor                                                      |

**Value**

A PharmacoSig object build from the provided signature data

**Examples**

```
PharmacoSig()
```

---

|                  |                                                       |
|------------------|-------------------------------------------------------|
| plot.PharmacoSig | <i>Plots a PharmacoSig object into a Volcano Plot</i> |
|------------------|-------------------------------------------------------|

---

**Description**

Given a PharmacoSig, this will plot a volcano plot, with parameters to set cutoffs for a significant effect size, p value, to pick multiple testing correction strategy, and to change point colors. Built on top of ggplot, it will return the plot object which can be easily customized as any other ggplot.

**Usage**

```
## S3 method for class 'PharmacoSig'
plot(
  x,
  adjust.method,
  drugs,
  features,
  effect_cutoff,
  signif_cutoff,
  color,
  ...
)
```

**Arguments**

|               |                                                                                                                                               |
|---------------|-----------------------------------------------------------------------------------------------------------------------------------------------|
| x             | PharmacoSig a PharmacoSig object, result of drugSensitivitySig or drugPerturbationSig                                                         |
| adjust.method | character(1) or logical(1) either FALSE for no adjustment, or one of the methods implemented by p.adjust. Defaults to FALSE for no correction |
| drugs         | character a vector of drug names for which to plot the estimated associations with gene expression                                            |
| features      | character a vector of features for which to plot the estimated associations with drug treatment                                               |
| effect_cutoff | the cutoff to use for coloring significant effect sizes.                                                                                      |
| signif_cutoff | the cutoff to use for coloring significance by p value or adjusted p values. Not on log scale.                                                |
| color         | one color if no cutoffs set for plotting. A vector of colors otherwise used to color points the in three categories above.                    |
| ...           | additional arguments, not currently used, but left here for consistency with plot                                                             |

**Value**

returns a ggplot object, which by default will be evaluated and the plot displayed, or can be saved to a variable for further customization by adding ggplot elements to the returned graph

**Examples**

```
data(GDSCsmall)
drug.sensitivity <- drugSensitivitySig(GDSCsmall, mDataType="rna",
                                     nthread=1, features = fNames(GDSCsmall, "rna")[1])
plot(drug.sensitivity)
```

---

show,PharmacoSet-method

*Show a PharamcoSet*


---

**Description**

Show a PharamcoSet

**Usage**

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

**Arguments**

|        |             |
|--------|-------------|
| object | PharmacoSet |
|--------|-------------|

**Value**

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

@importFrom CoreGx show @importFrom methods callNextMethod

**Examples**

```
data(CCLEsmall)
CCLEsmall
```

---

```
show,PharmacoSig-method
```

*Show PharmacoGx Signatures*

---

**Description**

Show PharmacoGx Signatures

**Usage**

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

**Arguments**

object                  PharmacoSig

**Value**

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

**Examples**

```
data(GDSCsmall)
drug.sensitivity <- drugSensitivitySig(GDSCsmall, mDataType="rna",
                                     nthread=1, features = fNames(GDSCsmall, "rna")[1])
drug.sensitivity
```

---

`showSigAnnot,PharmacoSig-method`*Show the Annotations of a signature object*

---

## Description

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

## Usage

```
## S4 method for signature 'PharmacoSig'
showSigAnnot(object)
```

## Arguments

|        |                                                                                              |
|--------|----------------------------------------------------------------------------------------------|
| object | An object of the PharmacoSig Class, as returned by drugPerturbationSig or drugSensitivitySig |
|--------|----------------------------------------------------------------------------------------------|

## Value

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

## Examples

```
data(GDSCsmall)
drug.sensitivity <- drugSensitivitySig(GDSCsmall, mDataType="rna",
                                     nthread=1, features = fNames(GDSCsmall, "rna")[1])
showSigAnnot(drug.sensitivity)
```

---

`subsetTo,PharmacoSet-method`*A function to subset a PharmacoSet to data containing only specified drugs, cells and genes*

---

## Description

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

**Usage**

```
## S4 method for signature 'PharmacoSet'
subsetTo(
  object,
  cells = NULL,
  drugs = NULL,
  molecular.data.cells = NULL,
  keep.controls = TRUE,
  ...
)
```

**Arguments**

|                                   |                                                                                                                                                         |
|-----------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------|
| <code>object</code>               | A <code>PharmacoSet</code> to be subsetted                                                                                                              |
| <code>cells</code>                | A list or vector of cell names as used in the dataset to which the object will be subsetted. If left blank, then all cells will be left in the dataset. |
| <code>drugs</code>                | A list or vector of drug names as used in the dataset to which the object will be subsetted. If left blank, then all drugs will be left in the dataset. |
| <code>molecular.data.cells</code> | A list or vector of cell names to keep in the molecular data                                                                                            |
| <code>keep.controls</code>        | If the dataset has perturbation type experiments, should the controls be kept in the dataset? Defaults to true.                                         |
| <code>...</code>                  | Other arguments passed by other function within the package                                                                                             |

**Value**

A `PharmacoSet` with only the selected drugs and cells

**Examples**

```
data(CCLEsmall)
CCLEdrugs <- treatmentNames(CCLEsmall)
CCLEcells <- sampleNames(CCLEsmall)
pSet <- subsetTo(CCLEsmall, drugs = CCLEdrugs[1], cells = CCLEcells[1])
pSet
```

---

summarizeMolecularProfiles,PharmacoSet-method

*Takes molecular data from a PharmacoSet, and summarises them into one entry per drug*

---

**Description**

Given a `PharmacoSet` with molecular data, this function will summarize the data into one profile per cell line, using the chosen `summary.stat`. Note that this does not really make sense with perturbation type data, and will combine experiments and controls when doing the summary if run on a perturbation dataset.

**Usage**

```
## S4 method for signature 'PharmacoSet'
summarizeMolecularProfiles(
  object,
  mDataType,
  cell.lines,
  features,
  summary.stat = c("mean", "median", "first", "last", "and", "or"),
  fill.missing = TRUE,
  summarize = TRUE,
  verbose = TRUE,
  binarize.threshold = NA,
  binarize.direction = c("less", "greater"),
  removeTreated = TRUE
)
```

**Arguments**

|                                 |                                                                                                                                                                                                                 |
|---------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <code>object</code>             | PharmacoSet The PharmacoSet to summarize                                                                                                                                                                        |
| <code>mDataType</code>          | character which one of the molecular data types to use in the analysis, out of all the molecular data types available for the pset for example: rna, rnaseq, snp                                                |
| <code>cell.lines</code>         | character The cell lines to be summarized. If any cell.line has no data, missing values will be created                                                                                                         |
| <code>features</code>           | character A vector of the feature names to include in the summary                                                                                                                                               |
| <code>summary.stat</code>       | character which summary method to use if there are repeated cell.lines? Choices are "mean", "median", "first", or "last" In case molecular data type is mutation or fusion "and" and "or" choices are available |
| <code>fill.missing</code>       | boolean should the missing cell lines not in the molecular data object be filled in with missing values?                                                                                                        |
| <code>summarize</code>          | A flag which when set to FALSE (defaults to TRUE) disables summarizing and returns the data unchanged as a ExpressionSet                                                                                        |
| <code>verbose</code>            | boolean should messages be printed                                                                                                                                                                              |
| <code>binarize.threshold</code> | numeric A value on which the molecular data is binarized. If NA, no binarization is done.                                                                                                                       |
| <code>binarize.direction</code> | character One of "less" or "greater", the direction of binarization on binarize.threshold, if it is not NA.                                                                                                     |
| <code>removeTreated</code>      | logical If treated/perturbation experiments are present, should they be removed? Defaults to yes.                                                                                                               |

**Value**

`matrix` An updated PharmacoSet with the molecular data summarized per cell line.

## Examples

```
data(GDSCsmall)
GDSCsmall <- summarizeMolecularProfiles(GDSCsmall, mDataType = "rna", cell.lines=sampleNames(GDSCsmall), summary.
GDSCsmall
```

---

```
summarizeSensitivityProfiles,PharmacoSet-method
```

*Takes the sensitivity data from a PharmacoSet, and summarises them into a drug vs cell line table*

---

## Description

This function creates a table with cell lines as rows and drugs as columns, summarising the drug sensitivity data of a PharmacoSet into drug-cell line pairs

## Usage

```
## S4 method for signature 'PharmacoSet'
summarizeSensitivityProfiles(
  object,
  sensitivity.measure = "auc_recomputed",
  cell.lines,
  profiles_assay = "profiles",
  treatment_col = "treatmentid",
  sample_col = "sampleid",
  drugs,
  summary.stat = c("mean", "median", "first", "last", "max", "min"),
  fill.missing = TRUE,
  verbose = TRUE
)
```

## Arguments

|                     |                                                                                                                                                                         |
|---------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| object              | <a href="#">PharmacoSet</a> The PharmacoSet from which to extract the data                                                                                              |
| sensitivity.measure | <a href="#">character</a> The sensitivity measure to use. Use the <a href="#">sensitivityMeasures</a> function to find out what measures are available for each object. |
| cell.lines          | <a href="#">character</a> The cell lines to be summarized. If any cell lines have no data, they will be filled with missing values.                                     |
| profiles_assay      | <a href="#">character</a> The name of the assay in the PharmacoSet object that contains the sensitivity profiles.                                                       |
| treatment_col       | <a href="#">character</a> The name of the column in the profiles assay that contains the treatment IDs.                                                                 |
| sample_col          | <a href="#">character</a> The name of the column in the profiles assay that contains the sample IDs.                                                                    |

|              |                                                                                                                                                              |
|--------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------|
| drugs        | <b>character</b> The drugs to be summarized. If any drugs have no data, they will be filled with missing values.                                             |
| summary.stat | <b>character</b> The summary method to use if there are repeated cell line-drug experiments. Choices are "mean", "median", "first", "last", "max", or "min". |
| fill.missing | Should the missing cell lines not in the molecular data object be filled in with missing values?                                                             |
| verbose      | Should the function print progress messages?                                                                                                                 |

**Value**

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

**Examples**

```
data(GDSCsmall)
GDSCauc <- summarizeSensitivityProfiles(GDSCsmall,
  sensitivity.measure='auc_published')
```

---

updateObject,PharmacoSet-method

*Update the PharmacoSet class after changes in it struture or API*

---

**Description**

Update the PharmacoSet class after changes in it struture or API

**Usage**

```
## S4 method for signature 'PharmacoSet'
updateObject(object)
```

**Arguments**

object            A PharmacoSet object to update the class structure for.

**Value**

PharmacoSet with update class structure.

**Examples**

```
data(GDSCsmall)
updateObject(GDSCsmall)
```

---

```
[,PharmacoSet,ANY,ANY,ANY-method  
  [
```

---

**Description**

```
[
```

**Usage**

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

**Arguments**

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

**Value**

Returns the subsetting object

**Examples**

```
data(CCLEsmall)  
CCLEsmall["WM1799", "Sorafenib"]
```

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