

# Package ‘PharmacGx’

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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** Artistic-2.0

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'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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## R topics documented:

.computeLoewe	3
.effectToDose	4
.loewe	5
amcc	6
availablePSets	7
callingWaterfall	8
CCLEsmall	9
checkPsetStructure	9
CMAPsmall	10
computeABC	11
computeAmax	12
computeAUC	13
computeIC50	14
computeSlope	16
connectivityScore	17

cosinePerm . . . . . 18

dim,PharmacoSet-method . . . . . 19

downloadPertSig . . . . . 20

downloadPSet . . . . . 21

drugDoseResponseCurve . . . . . 22

drugPerturbationSig . . . . . 24

drugSensitivitySig,PharmacoSet-method . . . . . 25

filterNoisyCurves . . . . . 28

GDSCsmall . . . . . 29

geneDrugSensitivity . . . . . 29

geneDrugSensitivityPBCorr . . . . . 30

geneDrugSensitivityPCorr . . . . . 31

gwc . . . . . 32

HDAC\_genes . . . . . 33

intersectPSet . . . . . 34

logLogisticRegression . . . . . 35

mcc . . . . . 37

patialCorQUICKSTOP . . . . . 38

PharmacoSet . . . . . 39

PharmacoSet-accessors . . . . . 40

PharmacoSet-class . . . . . 50

PharmacoSet-utils . . . . . 51

PharmacoSet2 . . . . . 53

PharmacoSig . . . . . 54

plot.PharmacoSig . . . . . 55

show,PharmacoSet-method . . . . . 56

show,PharmacoSig-method . . . . . 56

showSigAnnot,PharmacoSig-method . . . . . 57

subsetTo,PharmacoSet-method . . . . . 58

summarizeSensitivityProfiles,PharmacoSet-method . . . . . 59

updateObject,PharmacoSet-method . . . . . 60

[,PharmacoSet,ANY,ANY,ANY-method . . . . . 60

**Index**

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

---

**Description**

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

**Usage**

```
.computeLoewe(
  viability,
  treatment1dose,
  treatment2dose,
  HS_1,
  HS_2,
  E_inf_1,
  E_inf_2,
  EC50_1,
  EC50_2
)
```

**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

`treatment2dose` numeric a vector of concentrations for treatment 2

`HS_1` numeric Hill coefficient of treatment 1

`HS_2` numeric Hill coefficient of treatment 2

`E_inf_1` numeric the maximum attainable effect of treatment 1.

`E_inf_2` numeric the maximum attainable effect of treatment 2.

`EC50_1` numeric relative EC50 of treatment 1.

`EC50_2` numeric relative EC50 of treatment 2.

**Value**

numeric expected viability under Loewe additive null assumption.

**Examples**

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

---

`.effectToDose` *Inverse function of Hill equation*

---

**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 from a response:  $f^{-1}(E) = EC50(\frac{1-E}{E-E_{inf}})^{\frac{1}{HS}}$

**Usage**

```
.effectToDose(viability, EC50, HS, E_inf)
```

**Arguments**

viability      numeric is a vector whose entries are the viability values in the range [0, 1].  
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.

**Value**

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

**Examples**

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

---

.loewe                              *Loewe Additive Combination Index (CI)*

---

**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**

```
.loewe(  
  viability,  
  treatment1dose,  
  HS_1,  
  E_inf_1,  
  EC50_1,  
  treatment2dose,  
  HS_2,  
  E_inf_2,  
  EC50_2  
)
```

**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.

**Value**

CI under Loewe additive definition

**Examples**

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

---

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**

x, y	Two paired vectors of values. Could be replicates of observations for the same experiments for example.
step.prct	Instead of testing all possible splits of the data, it is possible to test steps of a percentage size of the total number of ranks in x/y. If this variable is 0, function defaults to testing all possible splits.

min.cat	The minimum number of members per category. Classifications with less members fitting into both categories will not be considered.
nperm	The number of permutation to use for estimating significance. If 0, then no p-value is calculated.
nthread	Number of threads to parallelize 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))
```

---

availablePSets	<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**

canonical	logical(1) 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 PharmacoSet 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*

---

**Description**

A small example version of the CCLE PharmacoS, 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 object

**References**

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

---

checkPsetStructure

*A function to verify the structure of a PharmacoS*

---

**Description**

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

**Usage**

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

**Arguments**

<code>object</code>	A <code>PharmacoSet</code> to be verified
<code>plotDist</code>	Should the function also plot the distribution of molecular data?
<code>result.dir</code>	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)
```

---

`CMAPsmall`*Connectivity Map Example PharmacoSet*

---

**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	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 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 trapezoid numeric integral of the actual data provided. Alternatively, the parameters of a Hill Slope returned by logLogisticRegression can be passed in if they are 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)
```

---

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 `n`th percentile viability reduction

### Functions

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

### Examples

```

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

```

```
computeICn(dose, viability, n=10)
```

---

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)
```



---

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

x	factor is the factors for the first variable
y	factor is the factors for the second variable
nperm	integer is the number of permutations to compute the null distribution of MCC estimates
alternative	string indicates the alternative hypothesis and must be one of "two.sided", "greater" or "less". You can specify just the initial letter. "greater" corresponds to positive association, "less" to negative association. Options are 'two.sided', 'less', or 'greater'

include.perm    boolean indicates whether the estimates for the null distribution should be returned. Default set to 'FALSE'

nthread        integer is the number of threads to be used to perform the permutations in parallel

**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

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

---

## Description

This function allows you to download a PharmacoSet object for use with this package. The PharmacoSets have been extensively curated and organised within a PharmacoSet class, enabling use with all the analysis tools provided in PharmacoGx. 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 tempdir(). 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
)
```

**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.
trunc	logical(1) Should the viability values be truncated to lie in [0-100] before doing the fitting
legends.label	numeric A vector of sensitivity measurement types which could be any combination of ic50_published, auc_published, auc_recomputed and auc_recomputed_star. A legend will be displayed on the top right of the plot which each line of the legend is the values of requested sensitivity measurements for one of the requested pSets. If this parameter is missed no legend would be provided for the plot.
ylim	numeric A vector of two numerical values to be used as ylim of the plot. If this parameter would be missed c(0,100) would be used as the ylim of the plot.
xlim	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 concentrations between all the pSets would be used as plot xlim.
mycol	numeric A vector with the same length 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.
title	character The title of the graph. If no title is provided, then it defaults to 'Drug': 'Cell Line'.
plot.type	character Plot type which can be the actual one ("Actual") or the one fitted by log1 logistic regression ("Fitted") or both of them ("Both"). If this parameter is missed by default actual curve is plotted.
summarize.replicates	character If this parameter is set to true replicates are summarized and replicates are plotted individually otherwise
lwd	numeric The line width to plot with
cex	numeric The cex parameter passed to plot

cex.main            numeric The cex.main parameter passed to plot, controls the size of the titles  
 legend.loc         And argument passable to xy.coords for the position to place the legend.  
 verbose            logical(1) Should warning messages about the data passed in be printed?

### 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="22RV", pSets=GDSCsmall)
}

```

---

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

---

### 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, rnaseq, 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?

sensitivity.summary.stat	character	What summary statistic should be used to summarize duplicates for cell line sensitivity measurements?
returnValues	character	Which of estimate, t-stat, p-value and fdr should the function return for each gene drug pair?
sensitivity.cutoff	numeric	Allows the user to binarize the sensitivity data using this threshold.
standardize	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.
molecular.cutoff		Allows the user to binarize the sensitivity data using this threshold.
molecular.cutoff.direction	character	One of "less" or "greater", allows to set direction of binarization.
nthread	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)

```

---

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-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.

### Usage

```

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

```

### Arguments

pSet	<a href="#">PharmacoSet</a> a PharmacoSet object
epsilon	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
positive.cutoff.percent	numeric This value indicates that function may violate epsilon rule for how many points on drug-response curve
mean.viability	numeric average expected viability value
nthread	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)
```

---

`GDSCsmall`*Genomics of Drug Sensitivity in Cancer Example PharmacoS*

---

**Description**

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

**References**

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

---

`geneDrugSensitivity`*Calculate The Gene Drug Sensitivity*

---

**Description**

TODO:: Write a description!

**Usage**

```
geneDrugSensitivity(
  x,
  type,
  batch,
  drugpheno,
  interaction.typexgene = 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("PharmacGx_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**

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 <code>ceiling(1/req_alpha*100)</code> .
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::")
```

---

gwc

*GWC Score*

---

**Description**

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

**Usage**

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



**Arguments**

x1	numeric vector of effect sizes (e.g., fold change or t 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.

---

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 identifies to intersect on, drugs, cell lines, or concentrations
cells	a character vector of common cell lines between pSets. In case user is interested 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 interested 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, containing only the intersection

**Examples**

```

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

common$CGP
common$CCLE

```

---

**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**

<code>conc</code>	numeric is a vector of drug concentrations.
<code>viability</code>	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 <code>log_conc</code> , 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<sup>2</sup> 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<sup>2</sup> 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<sup>2</sup> 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 Matthews 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 entries 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)
```

---

patialCorQUICKSTOP      *QUICKSTOP significance testing for partial correlation*

---

### 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

```
patialCorQUICKSTOP(
  pin_x,
  pin_y,
  pobsCor,
  pGroupFactor,
  pGroupSize,
  pnumGroup,
  pMaxIter,
  pn,
  preq_alpha,
  ptolerance_par,
  plog_decision_boundary,
  pseed
)
```

### Arguments

pin_x	one of the two vectors to correlate.
pin_y	the other vector to calculate
pobsCor	the observed (partial) correlation between these variables
pGroupFactor	an integer vector labeling group membership, to correct for in the partial correlation. <b>NEEDS TO BE ZERO BASED!</b>
pGroupSize	an integer vector of size length(unique(pGroupFactor)), counting the number of members of each group (basically table(pGroupFactor)) as integer vector
pnumGroup	how many groups are there (len(pGroupSize))
pMaxIter	maximum number of iterations to do, as a REAL NUMBER
pn	length of x and y, as a REAL NUMBER
preq_alpha	the required alpha for significance
ptolerance_par	the tolerance region for quickstop. Suggested to be 1/100th of req_alpha'
plog_decision_boundary	log (base e) of 1/probability of incorrectly calling significance, as per quickstop paper (used to determine the log-odds)
pseed	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.

<code>treatment</code>	A <code>data.frame</code> containing annotations for all treatments profiled in the dataset. Must contain the mandatory <code>treatmentid</code> column which uniquely identifies each treatment in the object.
<code>sensitivityInfo</code>	A <code>data.frame</code> containing the information for the sensitivity experiments. Must contain a <code>'sampleid'</code> column with unique identifiers to each sample, matching the sample object and a <code>'treatmentid'</code> columns with unique identifiers for each treatment, matching the treatment object.
<code>sensitivityRaw</code>	A 3 Dimensional array containing the raw drug dose response data for the sensitivity experiments
<code>sensitivityProfiles</code>	<code>data.frame</code> containing drug sensitivity profile statistics such as IC50 and AUC
<code>sensitivityN, perturbationN</code>	A <code>data.frame</code> summarizing the available sensitivity/perturbation data
<code>curationSample, curationTissue, curationTreatment</code>	A <code>data.frame</code> mapping the names for samples, tissues and treatments used in the data set to universal identifiers used between different CoreSet objects
<code>datasetType</code>	A <code>character(1)</code> string of <code>'sensitivity'</code> , <code>'perturbation'</code> , or <code>'both'</code> detailing what type of data can be found in the CoreSet, for proper processing of the data
<code>verify</code>	<code>logical(1)</code> Should the function verify the CoreSet and print out any errors it finds after construction?
<code>...</code>	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 PharmacSet 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 PharmacSet object. Arguments:

- value: A list of data.frames, one for each type of curated identifier. For a PharmacSet 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 PharmacSet 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 PharmacSet 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 PharmacSet 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 PharmacSet 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 PharmacSet 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 PharmacSet object. More specifically, retrieve the @rowData slot from the SummarizedExperiment from the @molecularProfiles of a PharmacSet 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 PharmacSet 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 PharmacoSet 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 PharmacoSet.

- 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 PharmacoSet 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 PharmacoSet 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 PharmacoSet 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 PharmacoSet 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 PharmacoSet 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 containing the annotations for all the drugs profiled in the data set, across all data types

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

perturbation A list containing \$n, a data.frame summarizing the available perturbation data,

curation A list containing mappings for \$treatment, 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 PharmacoSet object.
perturbation	A deprecated slot in a PharmacoSet 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 PharmacoSet 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      *Plots a PharmacoSig object into a Volcano Plot*

---

### 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

object	A PharmacoSet to be subsetted
cells	A list or vector of cell names as used in the dataset to which the object will be subsetted. If left blank, then all cells will be left in the dataset.
drugs	A list or vector of drug names as used in the dataset to which the object will be subsetted. If left blank, then all drugs will be left in the dataset.
molecular.data.cells	A list or vector of cell names to keep in the molecular data
keep.controls	If the dataset has perturbation type experiments, should the controls be kept in the dataset? Defaults to true.
...	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

```

---

```
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,
  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	character which sensitivity measure to use? Use the <code>sensitivityMeasures</code> function to find out what measures are available for each object.
cell.lines	character The cell lines to be summarized. If any cell lines has no data, it will be filled with missing values
drugs	character The drugs to be summarized. If any drugs has no data, it will be filled with missing values
summary.stat	character which summary method to use if there are repeated cell line-drug experiments? Choices are "mean", "median", "first", or "last"
fill.missing	boolean should the missing cell lines not in the molecular data object be filled in with missing values?
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.

---

[,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 subsetted object

**Examples**

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

# Index

## \* datasets

- CCLsmall, 9
- CMAPsmall, 10
- GDSCsmall, 29
- HDAC\_genes, 33
- .PharmacoSet (PharmacoSet-class), 50
- .computeLoewe, 3
- .effectToDose, 4
- .loewe, 5
- [,PharmacoSet,ANY,ANY,ANY-method, 60
  
- amcc, 6
- annotation (PharmacoSet-accessors), 40
- annotation,PharmacoSet-method  
(PharmacoSet-accessors), 40
- annotation<- (PharmacoSet-accessors), 40
- annotation<-,PharmacoSet,list-method  
(PharmacoSet-accessors), 40
- availablePSets, 7
  
- callingWaterfall, 8
- CCLsmall, 9
- cellInfo (PharmacoSet-accessors), 40
- cellInfo,PharmacoSet-method  
(PharmacoSet-accessors), 40
- cellInfo<- (PharmacoSet-accessors), 40
- cellInfo<-,PharmacoSet,data.frame-method  
(PharmacoSet-accessors), 40
- cellName,PharmacoSet-method  
(PharmacoSet-accessors), 40
- cellNames (PharmacoSet-accessors), 40
- cellNames<- (PharmacoSet-accessors), 40
- cellNames<-,PharmacoSet,list-method  
(PharmacoSet-accessors), 40
- checkPsetStructure, 9
- CMAPsmall, 10
- computeABC, 11
- computeAmax, 12
- computeAUC, 13
- computeIC50, 14
  
- computeICn (computeIC50), 14
- computeSlope, 16
- connectivityScore, 17
- cosinePerm, 18
- curation (PharmacoSet-accessors), 40
- curation,PharmacoSet-method  
(PharmacoSet-accessors), 40
- curation<- (PharmacoSet-accessors), 40
- curation<-,PharmacoSet,list-method  
(PharmacoSet-accessors), 40
  
- datasetType (PharmacoSet-accessors), 40
- datasetType,PharmacoSet-method  
(PharmacoSet-accessors), 40
- datasetType<- (PharmacoSet-accessors),  
40
- datasetType<-,PharmacoSet,character-method  
(PharmacoSet-accessors), 40
- dateCreated (PharmacoSet-accessors), 40
- dateCreated,PharmacoSet-method  
(PharmacoSet-accessors), 40
- dateCreated<- (PharmacoSet-accessors),  
40
- dateCreated<-,PharmacoSet,character-method  
(PharmacoSet-accessors), 40
- dateCreated<-,PharmacoSet-method  
(PharmacoSet-accessors), 40
- dim,PharmacoSet-method, 19
- downloadPertSig, 20
- downloadPSet, 21
- drugDoseResponseCurve, 22
- drugInfo (PharmacoSet-accessors), 40
- drugInfo<- (PharmacoSet-accessors), 40
- drugNames (PharmacoSet-accessors), 40
- drugNames<- (PharmacoSet-accessors), 40
- drugPerturbationSig, 24
- drugSensitivitySig,PharmacoSet-method,  
25
  
- featureInfo (PharmacoSet-accessors), 40

- featureInfo,PharmacoSet-method  
(PharmacoSet-accessors), 40
- featureInfo<- (PharmacoSet-accessors),  
40
- featureInfo<- ,PharmacoSet,character ,data.frame-method  
(PharmacoSet-accessors), 40
- featureInfo<- ,PharmacoSet,character ,DataFrame-method  
(PharmacoSet-accessors), 40
- filterNoisyCurves, 28
- fNames (PharmacoSet-accessors), 40
- fNames,PharmacoSet,character-method  
(PharmacoSet-accessors), 40
- fNames<- (PharmacoSet-accessors), 40
- fNames<- ,PharmacoSet,character ,character-method  
(PharmacoSet-accessors), 40
  
- GDSCsmall, 29
- geneDrugSensitivity, 29
- geneDrugSensitivityPBCorr, 30
- geneDrugSensitivityPCorr, 31
- gwc, 32
  
- HDAC\_genes, 33
  
- intersectPSet, 34
  
- logLogisticRegression, 35
  
- matrix, 60
- mcc, 37
- mDataNames (PharmacoSet-accessors), 40
- mDataNames,PharmacoSet-method  
(PharmacoSet-accessors), 40
- mDataNames<- (PharmacoSet-accessors), 40
- mDataNames<- ,PharmacoSet,ANY-method  
(PharmacoSet-accessors), 40
- mDataNames<- ,PharmacoSet-method  
(PharmacoSet-accessors), 40
- molecularProfiles  
(PharmacoSet-accessors), 40
- molecularProfiles,PharmacoSet-method  
(PharmacoSet-accessors), 40
- molecularProfiles<-  
(PharmacoSet-accessors), 40
- molecularProfiles<- ,PharmacoSet,character ,character-method  
(PharmacoSet-accessors), 40
- molecularProfiles<- ,PharmacoSet,character ,missing ,matrix-method  
(PharmacoSet-accessors), 40
- molecularProfiles<- ,PharmacoSet,missing ,missing ,list-method  
(PharmacoSet-accessors), 40
- molecularProfiles<- ,PharmacoSet,missing ,missing ,MultiAssayExperiment-method  
(PharmacoSet-accessors), 40
- molecularProfilesSlot  
(PharmacoSet-accessors), 40
- molecularProfilesSlot,PharmacoSet-method  
(PharmacoSet-accessors), 40
- molecularProfilesSlot<-  
(PharmacoSet-accessors), 40
- molecularProfilesSlot<- ,PharmacoSet,list-method  
(PharmacoSet-accessors), 40
- molecularProfilesSlot<- ,PharmacoSet,list\_OR\_MAE-method  
(PharmacoSet-accessors), 40
- molecularProfilesSlot<-PharmacoSet,MultiAssayExperiment-method  
(PharmacoSet-accessors), 40
- molecularProfilesSlot,PharmacoSet-method  
(PharmacoSet-accessors), 40
  
- name (PharmacoSet-accessors), 40
- name,PharmacoSet-method  
(PharmacoSet-accessors), 40
- name<- (PharmacoSet-accessors), 40
- name<- ,PharmacoSet,character-method  
(PharmacoSet-accessors), 40
- name<- ,PharmacoSet-method  
(PharmacoSet-accessors), 40
  
- patialCorQUICKSTOP, 38
- pertNumber (PharmacoSet-accessors), 40
- pertNumber,PharmacoSet-method  
(PharmacoSet-accessors), 40
- pertNumber<- (PharmacoSet-accessors), 40
- pertNumber<- ,PharmacoSet,array-method  
(PharmacoSet-accessors), 40
- PharmacoSet, 25, 28, 39, 59
- PharmacoSet-accessors, 40
- PharmacoSet-class, 50
- PharmacoSet-utils, 51
- PharmacoSet2, 53
- PharmacoSig, 54
- phenoInfo (PharmacoSet-accessors), 40
- phenoInfo,PharmacoSet,character-method  
(PharmacoSet-accessors), 40
- phenoInfo<- (PharmacoSet-accessors), 40
- phenoInfo<- ,PharmacoSet,character ,data.frame-method  
(PharmacoSet-accessors), 40
- phenoInfo<- ,PharmacoSet,character ,DataFrame-method  
(PharmacoSet-accessors), 40
- plot.PharmaSig, 55

- sampleInfo (PharmacoSet-accessors), 40
- sampleInfo, PharmacoSet-method  
(PharmacoSet-accessors), 40
- sampleInfo<- (PharmacoSet-accessors), 40
- sampleInfo<- , PharmacoSet, data.frame-method  
(PharmacoSet-accessors), 40
- sampleName, PharmacoSet-method  
(PharmacoSet-accessors), 40
- sampleNames (PharmacoSet-accessors), 40
- sampleNames, PharmacoSet-method  
(PharmacoSet-accessors), 40
- sampleNames<- (PharmacoSet-accessors),  
40
- sampleNames<- , PharmacoSet, character-method  
(PharmacoSet-accessors), 40
- sampleNames<- , PharmacoSet, list-method  
(PharmacoSet-accessors), 40
- sensitivityInfo, PharmacoSet, character-method  
(PharmacoSet-accessors), 40
- sensitivityInfo, PharmacoSet, missing-method  
(PharmacoSet-accessors), 40
- sensitivityInfo, PharmacoSet-method  
(PharmacoSet-accessors), 40
- sensitivityInfo<- , PharmacoSet, data.frame-method  
(PharmacoSet-accessors), 40
- sensitivityInfo<- , PharmacoSet, missing, data.frame-method  
(PharmacoSet-accessors), 40
- sensitivityMeasures, PharmacoSet-method  
(PharmacoSet-accessors), 40
- sensitivityMeasures<- , PharmacoSet, character-method  
(PharmacoSet-accessors), 40
- sensitivityProfiles, PharmacoSet-method  
(PharmacoSet-accessors), 40
- sensitivityProfiles<- , PharmacoSet, data.frame-method  
(PharmacoSet-accessors), 40
- sensitivityRaw, PharmacoSet-method  
(PharmacoSet-accessors), 40
- sensitivityRaw<- , PharmacoSet, array-method  
(PharmacoSet-accessors), 40
- sensitivitySlot  
(PharmacoSet-accessors), 40
- sensitivitySlot<-  
(PharmacoSet-accessors), 40
- sensitivityInfo<- , PharmacoSet, character, data.frame-method  
(PharmacoSet-accessors), 40
- sensNumber (PharmacoSet-accessors), 40
- sensNumber , PharmacoSet-method  
(PharmacoSet-accessors), 40
- sensNumber<- (PharmacoSet-accessors), 40
- sensNumber<- , PharmacoSet, matrix-method  
(PharmacoSet-accessors), 40
- show, PharmacoSet-method, 56
- show, PharmacoSig-method, 56
- showSigAnnot, PharmacoSig-method, 57
- subsetByFeature (PharmacoSet-utils), 51
- subsetByFeature, PharmacoSet-method  
(PharmacoSet-utils), 51
- subsetBySample (PharmacoSet-utils), 51
- subsetBySample, CoreSet-method  
(PharmacoSet-utils), 51
- subsetBySample, PharmacoSet-method  
(PharmacoSet-utils), 51
- subsetByTreatment (PharmacoSet-utils),  
51
- subsetByTreatment, PharmacoSet-method  
(PharmacoSet-utils), 51
- subsetTo, PharmacoSet-method, 58
- summarizeSensitivityProfiles, PharmacoSet-method,  
59
- treatmentResponse<- , PharmacoSet, list-method  
(PharmacoSet-accessors), 40
- treatmentInfo (PharmacoSet-accessors),  
40
- treatmentInfo, PharmacoSet-method  
(PharmacoSet-accessors), 40
- treatmentInfo<-  
(PharmacoSet-accessors), 40
- treatmentInfo<- , PharmacoSet, data.frame-method  
(PharmacoSet-accessors), 40
- treatmentNames (PharmacoSet-accessors),  
40
- treatmentNames, PharmacoSet-method  
(PharmacoSet-accessors), 40
- treatmentNames<-  
(PharmacoSet-accessors), 40
- treatmentNames<- , PharmacoSet, character-method  
(PharmacoSet-accessors), 40
- treatmentResponse  
(PharmacoSet-accessors), 40
- treatmentResponse, PharmacoSet-method  
(PharmacoSet-accessors), 40
- treatmentResponse<-  
(PharmacoSet-accessors), 40
- treatmentResponse<- , PharmacoSet, list\_OR\_LongTable-method  
(PharmacoSet-accessors), 40



treatmentResponse<- ,PharmacoSet,LongTable-method  
(PharmacoSet-accessors), [40](#)

updateObject,PharmacoSet-method, [60](#)