

# Package ‘rcellminer’

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**Type** Package

**Title** rcellminer: Molecular Profiles and Drug Response for the NCI-60 Cell Lines

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**Author** Augustin Luna, Vinodh Rajapakse, Fabricio Sousa

**Maintainer**

Augustin Luna <lunaa@cbio.mskcc.org>, Vinodh Rajapakse <vinodh.rajapakse@nih.gov>

**Description** The NCI-60 cancer cell line panel has been used over the course of several decades as an anti-cancer drug screen. This panel was developed as part of the Developmental Therapeutics Program (DTP, <http://dtp.nci.nih.gov/>) of the U.S. National Cancer Institute (NCI). Thousands of compounds have been tested on the NCI-60, which have been extensively characterized by many platforms for gene and protein expression, copy number, mutation, and others (Reinhold, et al., 2012). The purpose of the CellMiner project (<http://discover.nci.nih.gov/cellminer>) has been to integrate data from multiple platforms used to analyze the NCI-60 and to provide a powerful suite of tools for exploration of NCI-60 data.

**License** LGPL-3

**LazyData** true

**Imports** stringr, gplots, methods, shiny

**Depends** R (>= 3.1.1), Biobase, rcdk, fingerprint

**Suggests** knitr, RColorBrewer, sqldf, BiocGenerics, testthat, rcellminerData, BiocStyle

**URL** <http://discover.nci.nih.gov/cellminer/>

**VignetteBuilder** knitr

**biocViews** aCGH, CellBasedAssays, CopyNumberVariation, GeneExpression, Pharmacogenomics, Pharmacogenetics, miRNA, Cheminformatics, Visualization, Software, SystemsBiology

**NeedsCompilation** no

**R topics documented:**

cmVersion . . . . .	3
compareFingerprints . . . . .	4
crossCors . . . . .	5
crossCorsSpearman . . . . .	5
DrugData . . . . .	6
DrugData,eSet,eSet,MIAXE-method . . . . .	7
DrugData-class . . . . .	7
drugDB . . . . .	8
elNetMolDataNCI60 . . . . .	9
fingerprintList . . . . .	10
getAct . . . . .	10
getAct,DrugData-method . . . . .	11
getActivityRangeStats . . . . .	11
getAllFeatureData . . . . .	12
getAllFeatureData,MolData-method . . . . .	12
getBinaryMutationData . . . . .	13
getColumnQuantiles . . . . .	14
getDrugActivityData . . . . .	14
getDrugActivityRange . . . . .	15
getDrugActivityRepeatData . . . . .	16
getDrugMoaList . . . . .	16
getDrugName . . . . .	17
getESetList . . . . .	18
getESetList,MolData-method . . . . .	18
getFeatureDataFromMatList . . . . .	19
getFingerprintList . . . . .	19
getMedSenLineActivity . . . . .	20
getMinDrugActivityRepeatCor . . . . .	21
getMoaStr . . . . .	22
getMoaToCompounds . . . . .	22
getMolDataMatrices . . . . .	23
getMolDataType . . . . .	23
getNumDrugActivityRepeats . . . . .	24
getNumMissingLines . . . . .	25
getRepeatAct . . . . .	25
getRepeatAct,DrugData-method . . . . .	26
getRsd . . . . .	26
getSampleData . . . . .	27
getSampleData,DrugData-method . . . . .	27
getSampleData,MolData-method . . . . .	28
getSmiles . . . . .	28
hasMoa . . . . .	29
initialize,DrugData-method . . . . .	29
initialize,MolData-method . . . . .	30
isPublic . . . . .	30
loadNciColorSet . . . . .	31

MolData . . . . .	31
MolData,list,MIAXE-method . . . . .	32
MolData-class . . . . .	32
passRuleOf5 . . . . .	33
passRuleOf5FromNsc . . . . .	34
patternComparison . . . . .	34
plotCellMiner . . . . .	35
plotDrugActivityRepeats . . . . .	36
plotDrugSets . . . . .	37
plotStructuresFromNscs . . . . .	38
rdkplot . . . . .	39
removeMolDataType . . . . .	39
restrictFeatureMat . . . . .	40
runShinyComparePlots . . . . .	41
runShinyCompareStructures . . . . .	41
runShinyCompoundBrowser . . . . .	42
selectCorrelatedRows . . . . .	42
selectCorrelatedRows2 . . . . .	43
[[,MolData-method . . . . .	44
[[<-,MolData-method . . . . .	44
<b>Index</b>	<b>46</b>

---

cmVersion

*CellMiner Version*


---

## Description

CellMiner Version

## Details

The version of CellMiner used

## Author(s)

Vinodh Rajapakse <vinodh.rajapakse AT nih.gov>

## References

<http://discover.nci.nih.gov/cellminer>

---

compareFingerprints     *Compare Structure Fingerprints to NCI DTP Compounds*

---

### Description

This function compares the first SMILES structure to all other structures given.

### Usage

```
compareFingerprints(ids = NULL, smiles = NULL, fpType = "standard",  
  verbose = TRUE, fingerprint.list = NULL)
```

### Arguments

ids	a vector of IDs corresponding to structures
smiles	a vector of strings SMILES structures
fpType	the type of fingerprint to be used; uses the RCDK <code>get.fingerprint()</code> (default: standard)
verbose	a boolean whether to display debugging information
fingerprint.list	a list of fingerprints generated with <code>getFingerprintList</code>

### Value

a sorted named vector of Tanimoto distances

### See Also

`rcdk::get.fingerprint`

### Examples

```
drugAnnot <- as(featureData(getAct(rcellminerData::drugData)), "data.frame")  
ids <- head(drugAnnot$NSC)  
smiles <- head(drugAnnot$SMILES)  
fingerprintList <- getFingerprintList(ids, smiles)  
compareFingerprints(fingerprint.list=fingerprintList)
```

---

crossCors	<i>Calculate cross-correlations with between rows of input matrices</i>
-----------	---

---

**Description**

Calculate cross-correlations with between rows of input matrices

**Usage**

```
crossCors(X, Y = NULL, method = "pearson")
```

**Arguments**

X	a matrix or data.frame
Y	a matrix or data.frame
method	a string specifying the type of correlation, chosen from pearson (default) or spearman.

**Value**

a list containing matrices of pairwise correlations and their p-values between rows of the input matrices or dataframes.

**Author(s)**

Sudhir Varma, NCI-LMP, with input checks, support for Spearman's correlation added by VNR.

**Examples**

```
drugActData <- exprs(getAct(rcellminerData::drugData))
crossCors(drugActData[c("94600"), ], drugActData[c("727625", "670655"), ])
crossCors(drugActData[c("94600"), ], drugActData[c("727625", "670655"), ], method="spearman")
```

---

crossCorsSpearman	<i>Calculate Spearman's correlations with between rows of input matrices</i>
-------------------	--

---

**Description**

Calculate Spearman's correlations with between rows of input matrices

**Usage**

```
crossCorsSpearman(X, Y = NULL)
```

**Arguments**

X	a matrix or data.frame
Y	a matrix or data.frame

**Value**

a list containing matrices of pairwise Spearman's correlations and their p-values between rows of the input matrices or dataframes.

**Examples**

```
## Not run:  
crossCorsSpearman(drugActData[c("94600"), ], drugActData[c("727625", "670655"), ])  
  
## End(Not run)
```

---

DrugData	<i>Returns a DrugData object.</i>
----------	-----------------------------------

---

**Description**

Returns a DrugData object.

**Usage**

```
DrugData(act, repeatAct, sampleData, ...)
```

**Arguments**

act	An eSet object containing drug activity data across a set of biological samples.
repeatAct	An eSet object containing repeat drug activity experiment data with respect to the same samples associated with act.
sampleData	A MIAxE object capturing sample and other data set information.
...	Other possible parameters.

**Value**

A DrugData object.

---

DrugData,eSet,eSet,MIAXE-method  
*Returns a DrugData object.*

---

**Description**

Returns a DrugData object.

**Usage**

```
## S4 method for signature 'eSet,eSet,MIAXE'
DrugData(act, repeatAct, sampleData, ...)
```

**Arguments**

act	An eSet object containing drug activity data across a set of biological samples.
repeatAct	An eSet object containing repeat drug activity experiment data with respect to the same samples associated with act.
sampleData	A MIAXE object capturing sample and other data set information.
...	Other possible parameters.

**Value**

A DrugData object.

---

DrugData-class	<i>An S4 class to represent drug activity and related data recorded for a set of biological samples.</i>
----------------	--

---

**Description**

An S4 class to represent drug activity and related data recorded for a set of biological samples.

**Arguments**

...	Other possible parameters.
-----	----------------------------

**Slots**

act	An eSet object containing drug activity data across a set of biological samples.
repeatAct	An eSet object containing repeat drug activity experiment data with respect to the same samples associated with act.
sampleData	A MIAXE object capturing sample and other data set information.

---

drugDB

*CellMiner Drug Response Values*

---

## Description

CellMiner Drug Response Values

## Details

A list containing response values and annotations:

- act Z-scores of the averaged negative log GI (growth inhibition) 50 values across repeats for the NCI-60; assay described here: <http://dtp.nci.nih.gov/branches/btb/ivclsp.html>
- annot
  - id Dataset identifier; NOTE: DO NOT use this column; the NSC is the primary drug identifier
  - nsc National Service Center identifier; the primary drug identifier
  - name Compound name
  - brand\_name Brand name for the compound, if sold commercially
  - formula Compound chemical formula
  - testing\_status Information on whether it is known if the compound is FDA approved or undergoing testing in clinical trials
  - source TODO
  - smiles Compound chemical structure as a SMILES string
  - weight Compound chemical weight in g/mol
  - mechanism Pharmacological mechanism of action
  - confidential\_flag A flag to indicate if compound information is public
  - total\_probes TODO
  - total\_good\_probes TODO
  - low\_correlations TODO
  - failure\_reason TODO
  - cas CAS Registry Number; NOTE: Due to data restrictions PubChem IDs are the preferred mapping ID to other datasets
  - pubchem\_id PubChem ID

## Author(s)

Vinodh Rajapakse <vinodh.rajapakse AT nih.gov>

## References

<http://discover.nci.nih.gov/cellminer/loadDownload.do>



## Description

Z-scores of values for a variety of assays conducted on the NCI-60 to facilitate comparison. Z-scores calculated over the 60 cell lines for the given feature.

## Details

A list containing various assay values:

- cop Copy number values; Described in Pubmed ID: 24670534
- exp Expression values; Obtained from "RNA: 5 Platform Gene Transcript" <http://discover.nci.nih.gov/cellminer/loadDownload.do>; Missing values imputed using the R package "impute"
- mut Mutation values; Deleterious mutations obtained from TODO
- mir MicroRNA values; Obtained from "RNA: Agilent Human microRNA (V2)" <http://discover.nci.nih.gov/cellminer/loadDownload.do>
- pro Reverse protein lysate array values; Obtain from "Protein: Lysate Array" <http://discover.nci.nih.gov/cellminer/loadDownload.do>
- mda NCI-60 metadata.
  - CNV\_GAIN Proportion of genome copy number gains; Described in Pubmed ID: 24670534
  - CNV\_LOSS Proportion of genome copy number losses; Described in Pubmed ID: 24670534
  - CNV\_TOTAL Sum of CNV\_GAIN and CNV\_LOSS
  - P53\_BIN Binary TP53 profile curated by William Reinhold
  - MSI\_OGAN\_BIN Binary microsatellite instability (MSI) profile curated by Ogan Abaan using COSMIC data; Obtained from Supplementary Table 1 - Ogan Whole Exome Sequencing (WES) paper in Cancer Res.
  - EPITHELIAL Epithelial by tissue of origin - pattern extracted from the CellMiner cell line metadata <http://discover.nci.nih.gov/cellminer/celllineMetadata.do>
  - EPITHELIAL\_KURT Kurt Kohn curation for epithelial-like cell lines based on molecular parameters described in Pubmed ID: 24940735
  - DELETTERIOUS Total deleterious variants from WES dataset; Fabricio Sousa curation
  - MISSENSE Total missense variants from WES dataset; Fabricio Sousa curation
  - SILENT Total silent variants from WES dataset; Fabricio Sousa curation
  - TOTAL\_AA Total amino acid changing variants from WES dataset; Fabricio Sousa curation
  - CELL-CELL Cell-to-cell adhesion curated by William Reinhold
  - DOUBLINGTIME The doubling time pattern was extracted from the CellMiner cell line metadata <http://discover.nci.nih.gov/cellminer/celllineMetadata.do>

## Author(s)

Vinodh Rajapakse <vinodh.rajapakse AT nih.gov>

**References**

<http://discover.nci.nih.gov/cellminer>

---

fingerprintList	<i>A list of pre-computed fingerprints using getFingerprintList()</i>
-----------------	---

---

**Description**

A list of pre-computed fingerprints using getFingerprintList()

---

getAct	<i>Returns an eSet object with drug activity data.</i>
--------	--

---

**Description**

Returns an eSet object with drug activity data.

**Usage**

```
getAct(object, ...)
```

**Arguments**

object	Object for which drug activity data is to be returned.
...	Other possible parameters.

**Value**

An eSet object with drug activity data.

---

getAct,DrugData-method

*Returns an eSet object with drug activity data.*

---

### Description

Returns an eSet object with drug activity data.

### Usage

```
## S4 method for signature 'DrugData'  
getAct(object)
```

### Arguments

object                    DrugData object for which drug activity data is to be returned.

### Value

An eSet object with drug activity data.

---

getActivityRangeStats *Returns a table of activity range statistics for a set of compounds.*

---

### Description

Returns a table of activity range statistics for a set of compounds.

### Usage

```
getActivityRangeStats(nscSet, concFormat = "NegLogGI50M",  
                      onlyCellMinerExps = TRUE)
```

### Arguments

nscSet                    a character vector specifying NSC identifier(s) for compound(s) of interest.

concFormat                a string selected from "NegLogGI50M" or "IC50MicroM". "NegLogGI50M" specifies activities as the negative log of the 50 inhibitory concentration (molar). "IC50MicroM" specifies activities as the 50 inhibitory concentration (micromolar).

onlyCellMinerExps        a logical value indicating whether to only return experimental data included in CellMiner (default=TRUE).

**Value**

a table of activity range statistics for a set of compounds.

**Examples**

```
nscSet <- c("609699", "740")
getActivityRangeStats(nscSet)
getActivityRangeStats(nscSet, concFormat="IC50MicroM")
```

---

getAllFeatureData      *Returns a list of feature data matrices.*

---

**Description**

Returns a list of feature data matrices.

**Usage**

```
getAllFeatureData(object, ...)
```

**Arguments**

object	Object for which a list of feature data matrices is to be returned.
...	Other possible parameters.

**Value**

A list of feature data matrices.

---

getAllFeatureData,MolData-method  
*Returns a list of feature data matrices.*

---

**Description**

Returns a list of feature data matrices.

**Usage**

```
## S4 method for signature 'MolData'
getAllFeatureData(object)
```

**Arguments**

object	MolData object for which a list of feature data matrices is to be returned.
--------	---

**Value**

A list of feature data matrices.

---

getBinaryMutationData *Compute a binary gene mutation data matrix from SNP and other mutation event-level data.*

---

## Description

Compute a binary gene mutation data matrix from SNP and other mutation event-level data.

## Usage

```
getBinaryMutationData(mutInfo, mutData, maxVariantFreq = 0.2,  
  maxNormalPopulationFreq = 0.005, maxSiftScore = 0.05,  
  minPolyPhenScore = 0.85)
```

## Arguments

- |                         |   |
|-------------------------|---|
| mutInfo                 | A data frame with the following named columns: Gene, the name of the gene associated with the mutation event; probe.ids, a unique identifier specifying the mutation event; SNP_1000_genome, the frequency of the mutation event in SNP 1000; ESP5400, the frequency of the mutation event in ESP5400; SNP_type, the type of mutation event, chosen from "MISSENSE", "FRAMESHIFT", "NON-FRAMESHIFT", "NONSENSE", "SPLICING"; SIFT_score, the SIFT score; Polyphen_score, the POLYPHEN score. Rownames of mutInfo should be set to probe.ids, i.e., the unique mutation event specifier. |
| mutData                 | A matrix with event level mutation information, with SNPs, etc. along rows and samples along columns. Rownames of mutData should exactly match those of mutInfo. The i-th row of mutInfo should thus give detailed information for the mutation event with data specified in the i-th row of mutData.   |
| maxVariantFreq          | The maximum proportion of mutant samples (used to exclude frequently occurring events); default value = 0.2.  |
| maxNormalPopulationFreq | The maximum frequency of a mutation in the normal population (used to exclude likely germline variants); default value = 0.005.   |
| maxSiftScore            | The maximum accepted SIFT score (used to exclude presumed non-deleterious mutations); default value = 0.05.   |
| minPolyPhenScore        | The minimum accepted POLYPHEN score (used to exclude presumed non-deleterious mutations); default value = 0.85.   |

## Value

A binary gene mutation matrix, with genes along rows, samples along columns, and 1s indicating deleterious mutations.

---

getColumnQuantiles      *Calculate quantile for the columns in a matrix*

---

**Description**

Calculate quantile for the columns in a matrix

**Usage**

```
getColumnQuantiles(X, prob, naRm = FALSE, onlyNonzeroVals = FALSE)
```

**Arguments**

X	the matrix
prob	a numeric probability
naRm	a boolean, whether to remove NAs
onlyNonzeroVals	a boolean, whether to only include non-zero values

**Value**

a vector of quantiles

**Examples**

```
getColumnQuantiles(matrix(1:25, nrow=5), prob = 0.5)
```

---

getDrugActivityData      *Returns a matrix containing activity (-logGI50) data for a set of compounds.*

---

**Description**

Returns a matrix containing activity (-logGI50) data for a set of compounds.

**Usage**

```
getDrugActivityData(nscSet, onlyCellMinerExps = TRUE)
```

**Arguments**

nscSet	A string specifying the NSC identifiers for the compounds.
onlyCellMinerExps	A logical value indicating whether to compute results using only experimental data included in CellMiner (default=TRUE).

**Value**

a matrix with NCI-60 average (over experiments)  $-\log_{GI50}$  activity data; compound activity profiles are along rows.

**Examples**

```
nscSet <- c("141540", "123127") # Etoposide, Doxorubicin.  
actData <- getDrugActivityData(nscSet)
```

---

getDrugActivityRange *Returns a vector of log activity range values for set of compounds.*

---

**Description**

Returns a vector of log activity range values for set of compounds.

**Usage**

```
getDrugActivityRange(nscSet, computeIQR = FALSE)
```

**Arguments**

nscSet	a character vector specifying NSC identifier(s) for compound(s) of interest.
computeIQR	logical value indicated whether inter-quartile range is to be computed; otherwise absolute range is computed (default=FALSE).

**Value**

a numeric vector of NCI-60 log activity ( $-\log_{GI50}$ ) range values indexed by the identifiers in nscSet.

**Examples**

```
nscSet <- c("609699", "740")  
getDrugActivityRange(nscSet)
```

---

getDrugActivityRepeatData

*Returns a matrix containing repeat activity experiment data for a compound.*

---

### Description

Returns a matrix containing repeat activity experiment data for a compound.

### Usage

```
getDrugActivityRepeatData(nscStr, concFormat = "NegLogGI50M",  
  onlyCellMinerExps = TRUE)
```

### Arguments

nscStr            a string specifying the NSC identifier for the compound.  
concFormat       a string selected from "NegLogGI50M" or "IC50MicroM". "NegLogGI50M" specifies activities as the negative log of the 50 inhibitory concentration (molar). "IC50MicroM" specifies activities as the 50 growth inhibitory concentration (micromolar).  
onlyCellMinerExps   a logical value indicating whether to only return experimental data included in CellMiner (default=TRUE).

### Value

a matrix with activity data from each experiment associated with a compound organized along the rows.

### Examples

```
nscStr <- "609699"  
actData <- getDrugActivityRepeatData(nscStr, concFormat='NegLogGI50M')  
actData <- getDrugActivityRepeatData(nscStr, concFormat='IC50MicroM')
```

---

getDrugMoaList

*Get a list of applicable MOA strings for a drug.*

---

### Description

Get a list of applicable MOA strings for a drug.

### Usage

```
getDrugMoaList(nsc, moaToCompoundListMap = NULL)
```



**Arguments**

nsc                    An NSC string.  
moaToCompoundListMap                    A named list of character vectors, with each name indicating an MOA class, and its corresponding character vector specifying MOA-associated drugs. If unspecified, this is constructed based on MOA information provided by CellMiner.

**Details**

[LINK TO MOAs?](#)

**Value**

A character vector giving all MOA classes for the drug.

**Examples**

```
getDrugMoaList("754365")
```

---

getDrugName	<i>Get the drug names for a set of NSC identifiers.</i>
-------------	---

---

**Description**

Get the drug names for a set of NSC identifiers.

**Usage**

```
getDrugName(nscSet)
```

**Arguments**

nscSet                    A character vector of NSC strings

**Value**

A named character vector indicating the compound names for each NSC in nscSet (with an empty string returned if no such information is available, and an NA returned if the NSC is not included in the CellMiner database).

**Examples**

```
nscSet <- c("609699", "94600")  
getDrugName(nscSet)
```

---

getESetList	<i>Returns a list of eSet objects.</i>
-------------	--

---

**Description**

Returns a list of eSet objects.

**Usage**

```
getESetList(object, ...)
```

**Arguments**

object	Object for which a list of eSets is to be returned.
...	Other possible parameters.

**Value**

A list of eSet objects.

---

getESetList,MolData-method	<i>Returns a list of eSet objects.</i>
----------------------------	--

---

**Description**

Returns a list of eSet objects.

**Usage**

```
## S4 method for signature 'MolData'  
getESetList(object)
```

**Arguments**

object	MolData object for which a list of eSet objects is to be returned.
--------	--

**Value**

A list of eSet objects.

---

`getFeatureDataFromMatList`

*Extract from a list of matrices the data associated with a set of features.*

---

**Description**

Extract from a list of matrices the data associated with a set of features.

**Usage**

```
getFeatureDataFromMatList(featureSet, dataMatList,  
  excludeMissingFeatures = TRUE)
```

**Arguments**

`featureSet` a character vector of feature names.  
`dataMatList` a list of matrices with feature data organized along the rows, and feature names accessible via `rownames(dataMatList)`.  
`excludeMissingFeatures` a logical value indicating whether features whose data cannot be found in any matrices in `dataMatList` should be excluded in the output. (default=TRUE).

**Value**

a single matrix containing data for all features in `featureSet`.

**Examples**

```
featureSet <- c("expSLFN11", "mutSLX4")  
molDataMats <- getMolDataMatrices()  
featureData <- getFeatureDataFromMatList(featureSet, molDataMats)
```

---

`getFingerprintList` *Get a list of fingerprints for a set of compounds*

---

**Description**

Get a list of fingerprints for a set of compounds

**Usage**

```
getFingerprintList(ids, smiles, fpType = "standard", verbose = TRUE)
```

**Arguments**

ids	a vector of IDs corresponding to structures
smiles	a vector of strings SMILES structures
fpType	the type of fingerprint to be used; uses the RCDK get.fingerprint() (default: standard)
verbose	show debugging output

**Value**

a list of fingerprints returned from RCDK where the list names are the IDs

**See Also**

rcdk::get.fingerprint

**Examples**

```
drugAnnot <- as(featureData(getAct(rcellminerData::drugData)), "data.frame")
ids <- head(drugAnnot$NSC)
smiles <- head(drugAnnot$SMILES)
fingerprintList <- getFingerprintList(ids, smiles)

## Not run:
# All fingerprints
ids <- drugAnnot$NSC
smiles <- drugAnnot$SMILES
fingerprintList <- getFingerprintList(ids, smiles)
save(fingerprintList, file="fingerprintList.RData")

## End(Not run)
```

---

getMedSenLineActivity *Returns a vector of median sensitive cell line activity (-logGI50) values for a set of compounds.*

---

**Description**

Returns a vector of median sensitive cell line activity (-logGI50) values for a set of compounds.

**Usage**

```
getMedSenLineActivity(idSet, senLineActZThreshold = 0.5,
  onlyCellMinerExps = TRUE, dataSource = "NCI60")
```

**Arguments**

`idSet` a character vector specifying identifier(s) for compound(s) of interest.  
`senLineActZThreshold` the minimum activity z-score for a sensitive cell line (default=0.5).  
`onlyCellMinerExps` a logical value indicating whether to base results strictly on experimental data included in CellMiner (default=TRUE).  
`dataSource` character string indicating data source (default="NCI60"). Currently only "NCI60" is supported.

**Value**

a numeric vector of median sensitive cell line activity (-logGI50) values indexed by the identifiers in `idSet`.

**Examples**

```
idSet <- c("609699", "740")
getMedSenLineActivity(idSet)
```

---

`getMinDrugActivityRepeatCor`

*Returns a table indicating, for each compound in a specified set, the least significant correlation and associated p-value between its replicate experiments.*

---

**Description**

Returns a table indicating, for each compound in a specified set, the least significant correlation and associated p-value between its replicate experiments.

**Usage**

```
getMinDrugActivityRepeatCor(nscSet)
```

**Arguments**

`nscSet` a character vector specifying NSC identifier(s) for compound(s) of interest.

**Value**

a dataframe containing the following columns: NSC, cor, pval

**Examples**

```
nscSet <- c("123528", "339316")
repExpCorTab <- getMinDrugActivityRepeatCor(nscSet)
```

---

getMoaStr	<i>Get MOA string</i>
-----------	-----------------------

---

**Description**

Get MOA string

**Usage**

```
getMoaStr(nscStr)
```

**Arguments**

nscStr            an NSC string

**Details**

LINK TO MOAs?

**Value**

a comma-delimited string with MOA

**Examples**

```
getMoaStr("94600")
```

---

getMoaToCompounds	<i>Get a named list mapping MOA classes to associated compound sets.</i>
-------------------	--

---

**Description**

Get a named list mapping MOA classes to associated compound sets.

**Usage**

```
getMoaToCompounds()
```

**Value**

a named list mapping MOA classes to associated compound sets (each represented as a character vector).

**Examples**

```
moaToCompounds <- getMoaToCompounds()
```

---

getMolDataMatrices	<i>Returns a list of molecular data type matrices, with rownames in each matrix prefixed with a data type abbreviation.</i>
--------------------	---

---

**Description**

Returns a list of molecular data type matrices, with rownames in each matrix prefixed with a data type abbreviation.

**Usage**

```
getMolDataMatrices(molDataMats = NULL)
```

**Arguments**

molDataMats	A named list of molecular data type matrices with feature data specified along the rows, and feature names indicated in the row names.
-------------	--

**Value**

a list containing molecular data type matrices, with rownames in each matrix prefixed with a data type abbreviation, e.g., 'exp' for mRNA expression, etc. The matrix-specific data type abbreviations are derived from the names of molDataMats.

**Examples**

```
molDataMats <- getMolDataMatrices()
```

---

getMolDataType	<i>Get the molecular data type prefixes for a set of features.</i>
----------------	--

---

**Description**

Get the molecular data type prefixes for a set of features.

**Usage**

```
getMolDataType(features, prefixLen = 3)
```

**Arguments**

features	A vector of features.
prefixLen	The length of the molecular data type prefix.

**Value**

A character vector of molecular data type prefixes.

#'

**Examples**

```
getMolDataType(c("expTP53", "copMDM2", "mutCHEK2", "mutBRAF"))
```

---

```
getNumDrugActivityRepeats
```

*Returns a vector indicating the number of drug activity repeat experiments with available data for each member of a set of compounds.*

---

**Description**

Returns a vector indicating the number of drug activity repeat experiments with available data for each member of a set of compounds.

**Usage**

```
getNumDrugActivityRepeats(nscSet, onlyCellMinerExps = TRUE)
```

**Arguments**

nscSet a character vector specifying NSC identifier(s) for compound(s) of interest.

onlyCellMinerExps

a logical value indicating whether to return only the number of experiments with data included in CellMiner (default=TRUE).

**Value**

a numeric vector, indexed by nscSet, indicating the number of drug activity repeat experiments for each one of its compounds.

**Examples**

```
nscSet <- c("1", "17", "89", "609699")
getNumDrugActivityRepeats(nscSet)
```



---

getNumMissingLines      *Returns a vector indicating the number of NCI-60 cell lines with missing activity data for set of compounds.*

---

**Description**

Returns a vector indicating the number of NCI-60 cell lines with missing activity data for set of compounds.

**Usage**

```
getNumMissingLines(nscSet)
```

**Arguments**

nscSet                  a character vector specifying NSC identifier(s) for compound(s) of interest.

**Value**

a numeric vector indicating the number of NCI-60 cell lines with missing activity data, indexed by the identifiers in nscSet.

**Examples**

```
nscSet <- c("1", "17", "89", "609699")
getNumMissingLines(nscSet)
```

---

getRepeatAct              *Returns an eSet object with drug repeat activity experiment data.*

---

**Description**

Returns an eSet object with drug repeat activity experiment data.

**Usage**

```
getRepeatAct(object, ...)
```

**Arguments**

object                  Object for which drug repeat activity experiment data is to be returned.  
...                      Other possible parameters.

**Value**

An eSet object with drug repeat activity experiment data.

---

getRepeatAct, DrugData-method

*Returns an eSet object with drug repeat activity experiment data.*

---

### Description

Returns an eSet object with drug repeat activity experiment data.

### Usage

```
## S4 method for signature 'DrugData'
getRepeatAct(object)
```

### Arguments

object                    DrugData object for which drug repeat activity experiment data is to be returned.

### Value

An eSet object with drug repeat activity experiment data.

---

getRsd

*Computes the relative standard deviation values with respect to the columns of a matrix or data.frame.*

---

### Description

Computes the relative standard deviation values with respect to the columns of a matrix or data.frame.

### Usage

```
getRsd(dat, onlyReturnMedian = TRUE)
```

### Arguments

dat                    a matrix or data.frame with numeric values.  
 onlyReturnMedian    a logical value indicating whether only the median column RSD value should be returned (vs. all RSD values).

### Value

median RSD value over the data set columns or all RSD values, depending on value of onlyReturnMedian (default=TRUE).

**Examples**

```
A <- matrix(rnorm(10*60), nrow=10)
getRsd(A)
getRsd(A, onlyReturnMedian=FALSE)
```

---

getSampleData	Returns a data frame with sample information.
---------------	---

---

**Description**

Returns a data frame with sample information.

**Usage**

```
getSampleData(object, ...)
```

**Arguments**

object	Object for which sample data is to be returned.
...	Other possible parameters.

**Value**

A data frame with sample information.

---

getSampleData,DrugData-method	Returns a data frame with sample information.
-------------------------------	---

---

**Description**

Returns a data frame with sample information.

**Usage**

```
## S4 method for signature 'DrugData'
getSampleData(object)
```

**Arguments**

object	DrugData object for which sample data is to be returned.
--------	--

**Value**

A data frame with sample information.

---

getSampleData, MolData-method

*Returns a data frame with sample information.*

---

### Description

Returns a data frame with sample information.

### Usage

```
## S4 method for signature 'MolData'  
getSampleData(object)
```

### Arguments

object            MolData object for which sample data is to be returned.

### Value

A data frame with sample information.

---

getSmiles

*Get the SMILES strings for a set of NSC identifiers.*

---

### Description

Get the SMILES strings for a set of NSC identifiers.

### Usage

```
getSmiles(nscSet)
```

### Arguments

nscSet            A character vector of NSC strings

### Value

A named character vector indicating the SMILES string for each NSC in nscSet (or NA if no structural information is available).

### Examples

```
nscSet <- c("609699", "94600")  
getSmiles(nscSet)
```

---

hasMoa	<i>Check if NSC has Mechanism of Action (MOA) Annotation</i>
--------	--

---

**Description**

Check if NSC has Mechanism of Action (MOA) Annotation

**Usage**

```
hasMoa(nsc)
```

**Arguments**

nsc	a string, an NSC identifier
-----	-----------------------------

**Value**

a boolean whether the NSC has an MOA

**Examples**

```
hasMoa("754365")
```

---

initialize,DrugData-method	<i>Returns a DrugData object.</i>
----------------------------	-----------------------------------

---

**Description**

Returns a DrugData object.

**Usage**

```
## S4 method for signature 'DrugData'
initialize(.Object, act, repeatAct, sampleData)
```

**Arguments**

.Object	An object: see "new()" documentation in "methods" package.
act	An eSet object containing drug activity data across a set of biological samples.
repeatAct	An eSet object containing repeat drug activity experiment data with respect to the same samples associated with act.
sampleData	A MIAxE object capturing sample and other data set information.

**Value**

A DrugData object.

**Note**

Seems to be required for definition of a constructor.

---

initialize, MolData-method

*Returns a MolData object.*

---

**Description**

Returns a MolData object.

**Usage**

```
## S4 method for signature 'MolData'  
initialize(.Object, eSetList, sampleData)
```

**Arguments**

.Object	An object: see "new()" documentation in "methods" package.
eSetList	A list of eSet objects for a common set of samples.
sampleData	A MIAxE object capturing sample and other data set information.

**Value**

A MolData object.

---

isPublic

*Check if an NSC ID is public*

---

**Description**

Check if an NSC ID is public

**Usage**

```
isPublic(nscs)
```

**Arguments**

nscs	a vector of NSC string IDs
------	----------------------------

**Value**

a vector of boolean values of whether each NSC is public

**Examples**

```
isPublic("-1")  
isPublic(c("-1", "609699"))
```

---

loadNciColorSet	<i>Returns a 60-element color set that matches the color set used on <a href="http://discover.nci.nih.gov/">http://discover.nci.nih.gov/</a></i>
-----------------	--

---

**Description**

Returns a 60-element color set that matches the color set used on <http://discover.nci.nih.gov/>

**Usage**

```
loadNciColorSet(returnDf = FALSE)
```

**Arguments**

returnDf	a boolean if a data.frame with tissue names and abbreviations should be returned (default: FALSE)
----------	---

**Value**

a vector of colors as strings or a data.frame with tissues, tissue abbreviations, cell line abbreviations and colors

**Examples**

```
loadNciColorSet()
```

---

MolData	<i>Returns a MolData object.</i>
---------	----------------------------------

---

**Description**

Returns a MolData object.

**Usage**

```
MolData(eSetList, sampleData, ...)
```

**Arguments**

eSetList	A list of eSet objects for a common set of samples.
sampleData	A MIAxE object capturing sample and other data set information.
...	Other possible parameters.

**Value**

A MolData object.

---

MolData, list, MIAxE-method  
*Returns a MolData object.*

---

**Description**

Returns a MolData object.

**Usage**

```
## S4 method for signature 'list,MIAxE'
MolData(eSetList, sampleData, ...)
```

**Arguments**

eSetList	A list of eSet objects for a common set of samples.
sampleData	A MIAxE object capturing sample and other data set information.
...	Other possible parameters.

**Value**

A MolData object.

---

MolData-class      *An S4 class to represent molecular data recorded for a set of biological samples.*

---

**Description**

An S4 class to represent molecular data recorded for a set of biological samples.

**Arguments**

...      Other possible parameters.



**Slots**

eSetList A list of eSet objects for a common set of samples.  
 sampleData A MIAxE object capturing sample and other data set information.

---

passRuleOf5	<i>Checks if SMILES passes Lipinski's Rule of 5</i>
-------------	---

---

**Description**

Checks if SMILES passes Lipinski's Rule of 5

**Usage**

```
passRuleOf5(smiles, acceptableViolations = 0, verbose = FALSE)
```

**Arguments**

smiles a string, the SMILES structure to be checked  
 acceptableViolations, a number, the number of acceptable rule violations (default: 0)  
 verbose a boolean, whether to write out the failing criteria (default: FALSE)

**Details**

Uses RCDK: `org.openscience.cdk.qsar.descriptors.molecular.RuleOfFiveDescriptor`

**Value**

a boolean, whether the SMILES passes the criteria

**Examples**

```
# Docetaxel
passRuleOf5("CC1=C2C(C(=O)C3(C(CC4C(C3C(C(C2(C)C)CC1OC(=O)C(C(C5=CC=CC=C5)NC(=O)OC(C)(C)C)O)OC(=O)C6=CC=CC=C6)(C04)OC(=O)C)O)C)O", verbose=TRUE)

# Gemcitabine
passRuleOf5("C1=CN(C(=O)N=C1N)C2C(C(C(O2)CO)O)(F)F", verbose=TRUE)
```

---

passRuleOf5FromNsc      *Checks if NSC passes Lipinski's Rule of 5*

---

**Description**

Checks if NSC passes Lipinski's Rule of 5

**Usage**

```
passRuleOf5FromNsc(nsc, acceptableViolations = 0, verbose = FALSE)
```

**Arguments**

nsc                    a string, the NSC identifier to be checked  
acceptableViolations,  
                         a number, the number of acceptable rule violations (default: 0)  
verbose                a boolean, whether to write out the failing criteria (default: FALSE)

**Details**

Uses RCDK: org.openscience.cdk.qsar.descriptors.molecular.RuleOfFiveDescriptor

**Value**

a boolean or NA, whether the NSC passes the criteria or NA if the NSC had no structure

**Examples**

```
passRuleOf5FromNsc("94600", verbose=TRUE)
```

---

patternComparison      *Compare an input pattern against a set of patterns.*

---

**Description**

Compare an input pattern against a set of patterns.

**Usage**

```
patternComparison(pattern, profileMatrixList, method = "pearson")
```

**Arguments**

pattern	An N element input pattern specified as either a named vector or an 1 x N matrix or data frame. Names (or column names) must match the column names of each element of profileMatrixList.
profileMatrixList	A single matrix (or data frame) or a list of matrices (or data frames). Each matrix (data frame) must be k x N - that is the k patterns for comparison with the input pattern must be specified along the rows, with rownames set appropriately.
method	a string specifying the type of correlation, chosen from pearson (default) or spearman.

**Value**

A data frame with pattern comparison results. Specifically, if M is the total number patterns in profileMatrixList elements, an M x 2 matrix is returned with sorted Pearson's correlations in the first column and corresponding p-values in the second column. Comparison pattern names are indicated in the row names.

**Examples**

```
drugAct <- exprs(getAct(rcellminerData::drugData))
molDataMats <- getMolDataMatrices()[c("exp", "mut")]
molDataMats <- lapply(molDataMats, function(X) X[1:10, ])
pcResults <- patternComparison(drugAct["609699", ], molDataMats)
pcResults <- patternComparison(drugAct["609699", ], molDataMats, method="spearman")
pcResults <- patternComparison(drugAct["609699", ], molDataMats$exp, method="spearman")
```

---

plotCellMiner

*Description: Produces CellMiner-like plots in R*


---

**Description**

Description: Produces CellMiner-like plots in R

**Usage**

```
plotCellMiner(drugAct, molData, plots, nsc = NULL, gene = NULL,
  sub = NULL, xLimits = c(-3, 3), xLabel = "Z-scores", verbose = FALSE)
```

**Arguments**

drugAct	a matrix of drug activity values (cell lines as columns, drug entries as rows)
molData	a list of matrices a molecular
plots	a vector of characters denoting the plots to include and the order (e.g. c("mut", "drug", "cop"). Currently, supported entries mutations (mut), drug activities (drug), copy number variations (cop)

nsc	a string NSC ID that will be plotted when a "drug" entry appears in the plots vector
gene	a string HUGO gene symbol for which the "mut", "cop", or "exp" plots will be produced if in plots vector
sub	a vector of strings with sub-titles for each plot
xLimits	a 2 number vector with the the minimum and maximum X-axis values (default: c(-3, 3))
xLabel	a string for the default X-axis label
verbose	a boolean to show debugging information

**Value**

None

**Author(s)**

Augustin Luna &lt;augustin AT mail.nih.gov&gt;

**Examples**

```
drugAct <- exprs(getAct(rcellminerData::drugData))
molDataMats <- getMolDataMatrices()
plotDataMats <- molDataMats[c("exp", "cop", "mut")]
plotCellMiner(drugAct, plotDataMats,
plots=c("mut", "drug", "cop"), nsc="94600", gene="TP53")
```

---

plotDrugActivityRepeats

*Plot NCI-60 drug activity profiles for repeat experiments.*


---

**Description**

Plot NCI-60 drug activity profiles for repeat experiments.

**Usage**

```
plotDrugActivityRepeats(nscStr, useZScore = FALSE, maxRepNum = 5,
pdfFilename = NULL, pdfWidth = 12, pdfHeight = 6)
```

**Arguments**

nscStr	a string specifying the NSC identifier for a compound.
useZScore	a boolean specifying whether to plot z-transformed data (as opposed to -logGI50 values).
maxRepNum	an integer specifying the maximum number of repeat experiments to plot.
pdfFilename	name of a PDF output
pdfWidth	width of the PDF (default: 12)
pdfHeight	height of the PDF (default: 6)

**Value**

NONE

**Examples**

```
plotDrugActivityRepeats("609699")
plotDrugActivityRepeats("609699", useZScore=TRUE, maxRepNum=3)
```

---

plotDrugSets	<i>Produces a barplot of the average values for a set of NSCs with a error bar (one standard deviation)</i>
--------------	---

---

**Description**

Produces a barplot of the average values for a set of NSCs with a error bar (one standard deviation)

**Usage**

```
plotDrugSets(drugAct, drugs, mainLabel = "", pdfFilename = NULL)
```

**Arguments**

drugAct	a matrix of drug activity values (cell lines as columns, drug entries as rows)
drugs	a vector of NSC IDs whose values will be averaged by cell line
mainLabel	a main label for the plot
pdfFilename	a string file name for a PDF plot, no file output will be produced if this is not provided

**Value**

no values are returned

**Examples**

```
drugAct <- exprs(getAct(rcellminerData::drugData))
drugs <- rownames(drugAct)[1:8]
plotDrugSets(drugAct, drugs, "Test")
```

---

plotStructuresFromNscs

*Plot the structures for NSCs*

---

### Description

Plot the structures for NSCs

### Usage

```
plotStructuresFromNscs(nscs, smiles, titleCex = 1, structSize = 300,  
  structAnnotPos = 50, mainLabel = "", rows = 1, cols = length(nscs))
```

### Arguments

nscs	a vector of strings of NSCs used as structure titles
smiles	a vector of strings where the strings are SMILES structures
titleCex	a number, the scaling factor for the title (default: 1)
structSize	a number, the size of the structure image (default: 200)
structAnnotPos	a number, how far above the structure to display the title (default: 50)
mainLabel	a string, the main plot label
rows	number of rows in figure (default: 1)
cols	number of columns in figure (default: input structures number)

### Details

The parameter nscs is used as a title, this function does not search for nscs, but works based off the smiles given

### Value

the function does not return anything

### Author(s)

Augustin Luna <augustin AT mail.nih.gov>

### Examples

```
drugAnnot <- as(featureData(getAct(rcellminerData::drugData)), "data.frame")  
plotStructuresFromNscs("94600", drugAnnot["94600", "SMILES"])  
plotStructuresFromNscs(c("609699", "94600"),  
  drugAnnot[c("609699", "94600"), "SMILES"], mainLabel=c("609699", "94600"))
```

---

`rcdkplot`*Plot molecules*

---

**Description**

Plot molecules in R plot window instead of separate Java window

**Usage**

```
rcdkplot(molecule, width = 300, height = 300, marg = 0, main = "")
```

**Arguments**

<code>molecule</code>	an RCDK molecule
<code>width</code>	an integer width of the molecule
<code>height</code>	an integer height of the molecule
<code>marg</code>	margin for all side of the plot (default: 0)
<code>main</code>	a string the main title of the figure

**Details**

Code taken from: <http://www.cureffi.org/2013/09/23/a-quick-intro-to-chemical-informatics-in-r/>

**Value**

None

**Examples**

```
tmp <- parse.smiles("C1=CN(C(=O)N=C1N)C2C(C(C(O2)CO)O)(F)F")
rcdkplot(tmp[[1]], width=300, height=300, main="Gemcitabine")
```

---

`removeMolDataType`*Remove molecular data type prefixes from features.*

---

**Description**

Remove molecular data type prefixes from features.

**Usage**

```
removeMolDataType(features, prefixLen = 3)
```

**Arguments**

features            A vector of features.  
 prefixLen         The length of the molecular data type prefix.

**Details**

This function is primarily used to remove prefixes from elastic net features.

**Value**

A named vector of features without molecular data type prefixes.

**Examples**

```
removeMolDataType(c("expTP53", "copMDM2", "mutCHEK2", "mutBRAF"))
```

---

restrictFeatureMat	<i>Restricts a feature matrix to only include features associated with a specified gene set.</i>
--------------------	--

---

**Description**

Restricts a feature matrix to only include features associated with a specified gene set.

**Usage**

```
restrictFeatureMat(geneSet, featureMat, prefixSet = c("cop", "exp", "mut"))
```

**Arguments**

geneSet            a character vector of gene names.  
 featureMat        a matrix or data frame with feature vectors along rows and feature names specified in rownames(featureMat).  
 prefixSet         a set of feature name prefixes to be prepended to each element of geneSet to obtain a collection of geneSet-associated features.

**Value**

a matrix containing the features in the intersection of rownames(featureMat) and the set of geneSet-derived features (obtained by prepending each element of prefixSet to each gene in geneSet).

#'

**Examples**

```
X <- matrix(1:25, nrow=5)
rownames(X) <- c("expA", "expB", "copC", "mutC", "expD")
restrictFeatureMat(geneSet = c("B", "C"), X)
```



---

`runShinyComparePlots` *Run the Compare Plots Shiny App*

---

**Description**

Run the Compare Plots Shiny App

**Usage**

```
runShinyComparePlots(launch.browser = TRUE, port = 3838)
```

**Arguments**

`launch.browser` launch in browser? (default: TRUE)  
`port` port number to use

**Value**

None

**Examples**

```
port <- 3838  
# Uncomment first  
#runShinyComparePlots(port=port)
```

---

`runShinyCompareStructures`  
*Run the Compare Structures Shiny App*

---

**Description**

Run the Compare Structures Shiny App

**Usage**

```
runShinyCompareStructures(launch.browser = TRUE, port = 3838)
```

**Arguments**

`launch.browser` launch in browser? (default: TRUE)  
`port` port number to use

**Value**

None

**Examples**

```
port <- 3838
# Uncomment first
#runShinyCompareStructures(port=port)
```

---

```
runShinyCompoundBrowser
```

*Run the Compound Browser*

---

**Description**

Run the Compound Browser

**Usage**

```
runShinyCompoundBrowser(launch.browser = TRUE, port = 3838)
```

**Arguments**

launch.browser	launch in browser? (default: TRUE)
port	port number to use

**Value**

None

**Examples**

```
port <- 3838
# Uncomment first
#runShinyCompoundBrowser(port=port)
```

---

```
selectCorrelatedRows
```

*Get other features above some threshold*

---

**Description**

Get other features above some threshold

**Usage**

```
selectCorrelatedRows(Y, X, corThreshold = 0.1, useAbsCor = TRUE)
```

**Arguments**

Y	a vector or matrix; rows from X will be correlated with Y if Y is a vector or with rows of Y, if Y is a matrix.
X	a matrix of values that will be compared with Y (vector) or rows of Y (matrix)
corThreshold	the minimum correlation threshold for the row to be returned
useAbsCor	a logical value indicating whether absolute correlations should be used (default=TRUE).

**Value**

a matrix of rows of X correlated with Y (if Y is a vector) or correlated with at least one row of Y if Y is a matrix or data frame.

**Examples**

```
vec <- runif(10)
mat <- matrix(runif(100), 10, 10)
selectCorrelatedRows(vec, mat)
```

---

`selectCorrelatedRows2` *Get other features above some threshold (merges results from selectCorrelatedRows, invoked for a given Y, and each element in a list of matrices).*

---

**Description**

Get other features above some threshold (merges results from selectCorrelatedRows, invoked for a given Y, and each element in a list of matrices).

**Usage**

```
selectCorrelatedRows2(Y, XList, corThreshold = 0.1, useAbsCor = TRUE)
```

**Arguments**

Y	a vector or matrix; rows from each matrix element of X will be correlated with Y if Y is a vector or with rows of Y, if Y is a matrix.
XList	a list of matrices whose rows will be correlated with Y (vector) or rows of Y (matrix)
corThreshold	the minimum correlation threshold for the row to be returned
useAbsCor	a logical value indicating whether absolute correlations should be used (default=TRUE).

**Value**

a matrix formed from rows of matrices in XList that are correlated with Y (if Y is a vector) or correlated with at least one row of Y if Y is a matrix or data frame.

**Examples**

```
vec <- runif(10)
names(vec) <- 1:10
matList <- list(X1 = matrix(runif(100), 10, 10), X2 = matrix(runif(100), 10, 10))
rownames(matList$X1) <- paste0("X1_row_", 1:10)
colnames(matList$X1) <- paste0("X1_col_", 1:10)
rownames(matList$X2) <- paste0("X2_row_", 1:10)
colnames(matList$X2) <- paste0("X2_col_", 1:10)
selectCorrelatedRows2(vec, matList)
```

---

[[<-,MolData-method	<i>Returns an indexed eSet object from a MolData object eSet list.</i>
---------------------	--

---

**Description**

Returns an indexed eSet object from a MolData object eSet list.

**Usage**

```
## S4 method for signature 'MolData'
x[[i]]
```

**Arguments**

x	A MolData object.
i	Index or named item in MolData object eSet list.

**Value**

An indexed eSet object from a MolData object eSet list.

---

[[<-,MolData-method	<i>Assigns an eSet object to a specified position in a MolData object eSet list.</i>
---------------------	--

---

**Description**

Assigns an eSet object to a specified position in a MolData object eSet list.

**Usage**

```
## S4 replacement method for signature 'MolData'
x[[i]] <- value
```

**Arguments**

x	A MolData object.
i	Index or named item in MolData object eSet list.
value	An eSet object to be assigned.

**Value**

An eSet object to a specified position in a MolData object eSet list.

# Index

## \*Topic **data**

- cmVersion, 3
- drugDB, 8
- elNetMolDataNCI60, 9
- fingerprintList, 10
- .DrugData (DrugData-class), 7
- .MolData (MolData-class), 32
- [[, MolData-method, 44
- [[<- , MolData-method, 44
  
- cmVersion, 3
- compareFingerprints, 4
- crossCors, 5
- crossCorsSpearman, 5
  
- DrugData, 6
- DrugData, eSet, eSet, MIAxE-method, 7
- DrugData-class, 7
- drugDB, 8
  
- elNetMolDataNCI60, 9
  
- fingerprintList, 10
  
- getAct, 10
- getAct, DrugData-method, 11
- getActivityRangeStats, 11
- getAllFeatureData, 12
- getAllFeatureData, MolData-method, 12
- getBinaryMutationData, 13
- getColumnQuantiles, 14
- getDrugActivityData, 14
- getDrugActivityRange, 15
- getDrugActivityRepeatData, 16
- getDrugMoaList, 16
- getDrugName, 17
- getESetList, 18
- getESetList, MolData-method, 18
- getFeatureDataFromMatList, 19
- getFingerprintList, 19
- getMedSenLineActivity, 20
- getMinDrugActivityRepeatCor, 21
- getMoaStr, 22
- getMoaToCompounds, 22
- getMolDataMatrices, 23
- getMolDataType, 23
- getNumDrugActivityRepeats, 24
- getNumMissingLines, 25
- getRepeatAct, 25
- getRepeatAct, DrugData-method, 26
- getRsd, 26
- getSampleData, 27
- getSampleData, DrugData-method, 27
- getSampleData, MolData-method, 28
- getSmiles, 28
  
- hasMoa, 29
  
- initialize, DrugData-method, 29
- initialize, MolData-method, 30
- isPublic, 30
  
- loadNciColorSet, 31
  
- MolData, 31
- MolData, list, MIAxE-method, 32
- MolData-class, 32
  
- passRuleOf5, 33
- passRuleOf5FromNsc, 34
- patternComparison, 34
- plotCellMiner, 35
- plotDrugActivityRepeats, 36
- plotDrugSets, 37
- plotStructuresFromNscs, 38
  
- rcdkplot, 39
- removeMolDataType, 39
- restrictFeatureMat, 40
- runShinyComparePlots, 41
- runShinyCompareStructures, 41
- runShinyCompoundBrowser, 42

`selectCorrelatedRows`, [42](#)  
`selectCorrelatedRows2`, [43](#)