

Package ‘gDRtestData’

April 1, 2025

Title gDRtestData - R data package with testing dose response data

Version 1.5.1

Date 2024-11-05

Description R package with internal dose-response test data. Package provides functions to generate input testing data that can be used as the input for gDR pipeline. It also contains qs files with MAE data processed by gDR.

Depends R (>= 4.2)

Imports checkmate, data.table

Suggests BiocStyle, gDRstyle (>= 1.1.5), knitr, qs, reshape2, rmarkdown, SummarizedExperiment, testthat, yaml

URL <https://github.com/gdrplatform/gDRtestData>,
<https://gdrplatform.github.io/gDRtestData/>

BugReports <https://github.com/gdrplatform/gDRtestData/issues>

biocViews ExperimentData, TechnologyData

VignetteBuilder knitr

License Artistic-2.0

Encoding UTF-8

Roxygen list(markdown = TRUE)

RoxygenNote 7.3.1

Config/testthat/edition 3

git_url <https://git.bioconductor.org/packages/gDRtestData>

git_branch devel

git_last_commit 8be652c

git_last_commit_date 2024-11-06

Repository Bioconductor 3.21

Date/Publication 2025-04-01

Author Aleksander Chlebowski [aut],
 Bartosz Czech [aut] (ORCID: <<https://orcid.org/0000-0002-9908-3007>>),
 Arkadiusz Gladki [cre, aut] (ORCID:
 <<https://orcid.org/0000-0002-7059-6378>>),
 Marc Hafner [aut] (ORCID: <<https://orcid.org/0000-0003-1337-7598>>),
 Marcin Kamianowski [aut],
 Sergiu Mocanu [aut],
 Natalia Potocka [aut],
 Dariusz Scigocki [aut],
 Janina Smola [aut],
 Allison Young [aut]

Maintainer Arkadiusz Gladki <gladki.arkadiusz@gmail.com>

Contents

gDRtestData-package	2
add_concentration	3
add_data_replicates	4
add_day0_data	4
cell_lines	5
create_synthetic_cell_lines	5
create_synthetic_drugs	6
drugs	6
generate_ec50	7
generate_e_inf	7
generate_hill_coef	8
generate_response_data	8
get_test_dataset_paths	9
prepareCodilutionData	10
prepareComboMergedData	10
prepareData	11
prepareMergedData	12
Index	13

gDRtestData-package	<i>gDRtestData: gDRtestData - R data package with testing dose response data</i>
---------------------	--

Description

R package with internal dose-response test data. Package provides functions to generate input testing data that can be used as the input for gDR pipeline. It also contains qs files with MAE data processed by gDR.

Value

package help page

Note

To learn more about functions start with `help(package = "gDRtestData")`

Author(s)

Maintainer: Arkadiusz Gladki <gladki.arkadiusz@gmail.com> ([ORCID](#))

Authors:

- Aleksander Chlebowski
- Bartosz Czech ([ORCID](#))
- Marc Hafner ([ORCID](#))
- Marcin Kamianowski
- Sergiu Mocanu
- Natalia Potocka
- Dariusz Scigocki
- Janina Smola
- Allison Young

See Also

Useful links:

- <https://github.com/gdrplatform/gDRtestData>
- <https://gdrplatform.github.io/gDRtestData/>
- Report bugs at <https://github.com/gdrplatform/gDRtestData/issues>

add_concentration *Add concentrations*

Description

Add concentrations

Usage

```
add_concentration(df_layout, concentrations = 10^(seq(-3, 1, 0.5)))
```

Arguments

`df_layout` data.table that should contains the cell line, drug, concentration, and replicate columns along with the annotations that needs to be propagated

`concentrations` vector of numeric concentrations that will be added to `df_layout`

Value

data.table with concentrations

Examples

```
cell_lines <- create_synthetic_cell_lines()
add_concentration(cell_lines)
```

add_data_replicates *Add data replicates*

Description

Add data replicates

Usage

```
add_data_replicates(df_layout)
```

Arguments

df_layout data.table that should contains the cell line, drug, concentration, and replicate columns along with the annotations that needs to be propagated

Value

data.table with replicates

Examples

```
cell_lines <- create_synthetic_cell_lines()
add_data_replicates(cell_lines)
```

add_day0_data *Add data with day 0*

Description

Add data with day 0

Usage

```
add_day0_data(df_merged, noise_level = 0.05)
```

Arguments

df_merged data.table with merged data
noise_level numeric scalar with the level of noise added to the data

Value

data.table with day0 data

Examples

```
cell_lines <- create_synthetic_cell_lines()
drugs <- create_synthetic_drugs()
df_merged <- prepareData(cell_lines[seq_len(2), ], drugs[seq_len(4), ])
df_merged$Duration <- 72
df_merged$ReadoutValue <- 0
add_day0_data(df_merged)
```

cell_lines	<i>Cell lines</i>
------------	-------------------

Description

Cell lines

Value

data.table

Examples

```
path <- system.file("annotation_data", "cell_lines.csv", package = "gDRtestData")
data.table::fread(file = path)
```

create_synthetic_cell_lines	<i>Create data.table with synthetic cell lines</i>
-----------------------------	--

Description

Create data.table with synthetic cell lines

Usage

```
create_synthetic_cell_lines()
```

Value

data.table with synthetic cell lines

Examples

```
create_synthetic_cell_lines()
```

```
create_synthetic_drugs
```

Create data.table with synthetic drugs

Description

Create data.table with synthetic drugs

Usage

```
create_synthetic_drugs()
```

Value

data.table with synthetic drugs

Examples

```
create_synthetic_drugs()
```

drugs

Drugs

Description

Drugs

Value

data.table

Examples

```
path <- system.file("annotation_data", "drugs.csv", package = "gDRtestData")
data.table::fread(file = path)
```

generate_ec50	<i>Calculate EC50 metric</i>
---------------	------------------------------

Description

Calculate EC50 metric

Usage

```
generate_ec50(drugs, cell_lines)
```

Arguments

drugs	data.table with drugs
cell_lines	data.table with cell lines

Value

matrix with random EC50

Examples

```
generate_ec50(create_synthetic_drugs(), create_synthetic_cell_lines())
```

generate_e_inf	<i>Calculate E inf metric</i>
----------------	-------------------------------

Description

Calculate E inf metric

Usage

```
generate_e_inf(drugs, cell_lines)
```

Arguments

drugs	data.table with drugs
cell_lines	data.table with cell lines

Value

matrix with random E inf

Examples

```
generate_e_inf(create_synthetic_drugs(), create_synthetic_cell_lines())
```

```
generate_hill_coef
```

Generate hill coefficient

Description

Generate hill coefficient

Usage

```
generate_hill_coef(drugs, cell_lines)
```

Arguments

drugs	data.table with drugs
cell_lines	data.table with cell lines

Value

matrix with random hill coefficient

Examples

```
generate_hill_coef(create_synthetic_drugs(), create_synthetic_cell_lines())
```

```
generate_response_data
```

Generate response data

Description

Generate response data

Usage

```
generate_response_data(df_layout, noise_level = 0.1)
```

Arguments

df_layout	data.table that should contains the cell line, drug, concentration, and replicate columns along with the annotations that needs to be propagated
noise_level	numeric scalar with the level of noise added to the data

Value

data.table with response data

Examples

```
cell_lines <- create_synthetic_cell_lines()
drugs <- create_synthetic_drugs()
df_layout <- prepareData(cell_lines[seq_len(2), ], drugs[seq_len(4), ])
generate_response_data(df_layout)
```

`get_test_dataset_paths`
get_test_dataset_paths

Description

Returns named vector of absolute paths to test datasets.

Usage

```
get_test_dataset_paths(datasets_dir = NULL, pattern = "finalMAE_")
```

Arguments

`datasets_dir` path to directory with datasets (default NULL). If NULL, then `inst/testdata` directory from `gDRtestData` will be used.

`pattern` used to: (1) filter to `qs` files from the `dataset_dir` path and (2) prettify the labels of the files

Value

named vector of absolute paths

Author(s)

Kamil Foltynski <kamil.foltynski@contractors.roche.com>

Examples

```
get_test_dataset_paths()
path <- system.file("testdata", package = "gDRtestData", mustWork = TRUE)
get_test_dataset_paths(path)
```

prepareCodilutionData *prepareCodilutionData*

Description

Create data.table with input co-dilution data containing noise for testing purposes

Usage

```
prepareCodilutionData(  
  cell_lines,  
  drugs,  
  drugsIdx2 = 1,  
  conc = 10^(seq(-3, 1, 0.5)),  
  noise = 0.1  
)
```

Arguments

cell_lines	data.table with cell line info
drugs	data.table with drug info
drugsIdx2	numeric vector of ids for secondary drug (in drugs data.table)
conc	vector of doses
noise	number indicating level of noise

Value

data.table with input data for testing

Examples

```
prepareCodilutionData(create_synthetic_cell_lines()[seq_len(2), ],  
  create_synthetic_drugs()[seq_len(4), ])
```

prepareComboMergedData
prepareComboMergedData

Description

Create data.table with input combination data containing noise for testing purposes

Usage

```
prepareComboMergedData(
  cell_lines,
  drugs,
  drugsIdx1 = 2:4,
  drugsIdx2 = c(26, 26, 26),
  concentration = c(0, 0.2, 1),
  noise = 0.1,
  modifyDf2 = FALSE
)
```

Arguments

cell_lines	data.table with cell line info
drugs	data.table with drug info
drugsIdx1	numeric vector of ids for primary drug
drugsIdx2	numeric vector of ids for secondary drug
concentration	numeric vector of doses
noise	number indicating level of noise
modifyDf2	Boolean indicating if the table should be modified to keep reverse single agent data

Value

data.table with input data for testing

Examples

```
prepareComboMergedData(create_synthetic_cell_lines(), create_synthetic_drugs())
```

prepareData	<i>prepareData</i>
-------------	--------------------

Description

Create data.table with input data for testing purposes

Usage

```
prepareData(cell_lines, drugs, conc = 10^(seq(-3, 1, 0.5)))
```

Arguments

cell_lines	data.table with cell line info
drugs	data.table with drug info
conc	vector of doses

Value

data.table with input data for testing

Examples

```
prepareData(create_synthetic_cell_lines(), create_synthetic_drugs())
```

prepareMergedData	<i>prepareMergedData</i>
-------------------	--------------------------

Description

Create data.table with input data containing noise for testing purposes

Usage

```
prepareMergedData(cell_lines, drugs, noise = 0.1)
```

Arguments

cell_lines	data.table with cell line info
drugs	data.table with drug info
noise	number indicating level of noise

Value

data.table with input data for testing

Examples

```
prepareMergedData(create_synthetic_cell_lines(), create_synthetic_drugs())
```

Index

- * **data**
 - cell_lines, [5](#)
 - drugs, [6](#)
- * **generate_data**
 - add_concentration, [3](#)
 - add_data_replicates, [4](#)
 - add_day0_data, [4](#)
 - create_synthetic_cell_lines, [5](#)
 - create_synthetic_drugs, [6](#)
- * **generate_results**
 - generate_e_inf, [7](#)
 - generate_ec50, [7](#)
 - generate_hill_coef, [8](#)
 - generate_response_data, [8](#)
- * **generate_test_data**
 - get_test_dataset_paths, [9](#)
 - prepareCodilutionData, [10](#)
 - prepareComboMergedData, [10](#)
 - prepareData, [11](#)
 - prepareMergedData, [12](#)
- * **internal**
 - cell_lines, [5](#)
 - drugs, [6](#)
 - gDRtestData-package, [2](#)

[add_concentration, 3](#)

[add_data_replicates, 4](#)

[add_day0_data, 4](#)

[cell_lines, 5](#)

[create_synthetic_cell_lines, 5](#)

[create_synthetic_drugs, 6](#)

[drugs, 6](#)

[gDRtestData \(gDRtestData-package\), 2](#)

[gDRtestData-package, 2](#)

[generate_e_inf, 7](#)

[generate_ec50, 7](#)

[generate_hill_coef, 8](#)

[generate_response_data, 8](#)

[get_test_dataset_paths, 9](#)

[prepareCodilutionData, 10](#)

[prepareComboMergedData, 10](#)

[prepareData, 11](#)

[prepareMergedData, 12](#)