

# Package ‘gDRtestData’

May 16, 2024

**Title** gDRtestData - R data package with testing dose reponse data

**Version** 1.3.0

**Date** 2024-02-28

**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 (>= 1.1.3), 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** 7.3.0

**Config/testthat/edition** 3

**git\_url** <https://git.bioconductor.org/packages/gDRtestData>

**git\_branch** devel

**git\_last\_commit** f259c37

**git\_last\_commit\_date** 2024-04-30

**Repository** Bioconductor 3.20

**Date/Publication** 2024-05-16

**Author** Aleksander Chlebowski [aut],  
 Bartosz Czech [aut] (<<https://orcid.org/0000-0002-9908-3007>>),  
 Arkadiusz Gladki [cre, aut] (<<https://orcid.org/0000-0002-7059-6378>>),  
 Marc Hafner [aut] (<<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

<b>Index</b>	<b>13</b>
--------------	-----------

---

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>

Authors:

- Aleksander Chlebowski
- Bartosz Czech
- Marc Hafner
- Marcin Kamianowski
- Sergiu Mocanu
- Natalia Potocka
- Dariusz Scigocki
- Smola Janina
- Allison Vount

**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	<i>Add data replicates</i>
---------------------	----------------------------

---

**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	<i>Add data with day 0</i>
---------------	----------------------------

---

**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	<i>Generate hill coefficient</i>
--------------------	----------------------------------

---

**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	<i>Generate response data</i>
------------------------	-------------------------------

---

**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](#)