

# Package ‘gDRtestData’

December 11, 2025

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

**Version** 1.8.0

**Date** 2025-08-12

**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 (>= 1.7.1), 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

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

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**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](#))

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- 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>

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|                   |                           |
|-------------------|---------------------------|
| add_concentration | <i>Add concentrations</i> |
|-------------------|---------------------------|

---

**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 Foltyński <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
```

```
prepareData
```

---

**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())
```

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