

Package ‘gDRtestData’

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Title gDRtestData - R data package with testing dose response data

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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.

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

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| | |
|---------------------|--|
| 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)

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- Natalia Potocka
- Dariusz Scigocki
- Janina Smola
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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)

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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())
```

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