

Package ‘gDRcore’

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Description This package contains core functions to process and analyze drug response data. The package provides tools for normalizing, averaging, and calculation of gDR metrics data. All core functions are wrapped into the pipeline function allowing analyzing the data in a straightforward way.

License Artistic-2.0

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<https://gdrplatform.github.io/gDRcore/>

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Contents

gDRcore-package	3
.map_references	4
.standardize_conc	5
add_CellLine_annotation	6
add_Drug_annotation	7
add_intermediate_data	8
average_SE	9
calculate_excess	14
calculate_GR_value	15
calculate_matrix_metric	17
cleanup_metadata	19
convert_mae_to_raw_data	20
convert_se_to_raw_data	20
data_model	21
data_model.character	21
data_model.data.table	22
define_matrix_grid_positions	22
do_skip_step	23
fit_SE.combinations	23
generateCodilution	24
generateCodilutionSmall	25
generateComboMatrix	25
generateComboMatrixSmall	25
generateComboNoNoiseData	26

generateComboNoNoiseData2	26
generateComboNoNoiseData3	26
generateLigandData	27
generateMediumData	27
generateNoiseRawData	27
generateNoNoiseRawData	28
generateTripleComboMatrix	28
get_assays_per_pipeline_step	29
get_default_nested_identifiers	29
get_mae_from_intermediate_data	30
get_pipeline_steps	30
grr_matches	31
identify_data_type	32
identify_keys	34
is_preceding_step	35
map_conc_to_standardized_conc	35
map_df	36
map_ids_to_fits	38
map_untreated	39
merge_data	39
order_result_df	40
prepare_input	40
prepare_input.data.table	41
prepare_input.MultiAssayExperiment	42
read_intermediate_data	43
remove_drug_batch	44
replace_conc_with_standardized_conc	44
round_concentration	45
save_intermediate_data	46
split_raw_data	46
test_synthetic_data	48

Index	50
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gDRcore-package	<i>gDRcore: Processing functions and interface to process and analyze drug dose-response data</i>
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Description

This package contains core functions to process and analyze drug response data. The package provides tools for normalizing, averaging, and calculation of gDR metrics data. All core functions are wrapped into the pipeline function allowing analyzing the data in a straightforward way.

Value

package help page

Note

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

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See Also

Useful links:

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

.map_references

Map references

Description

Map references

Usage

```
.map_references(  
  mat_elem,  
  rowData_colnames = c(gDRutils::get_env_identifiers("duration"), paste0(c("drug",  
    "drug_name", "drug_moa"), "3"))  
)
```

Arguments

mat_elem input data frame
rowData_colnames character vector of variables for the mapping of reference treatments

Details

Using the given rownames, map the treated and reference conditions.

Value

list

`.standardize_conc` *Standardize concentration values.*

Description

Standardize concentration values.

Usage

```
.standardize_conc(conc)
```

Arguments

conc numeric vector of the concentrations

Details

If no conc are passed, NULL is returned.

Value

vector of standardized concentrations

Examples

```
concs <- 10 ^ (seq(-1, 1, 0.9))
.standardize_conc(concs)
```

```
add_CellLine_annotation
      add_CellLine_annotation
```

Description

add cellline annotation to a data.table with metadata

Usage

```
add_CellLine_annotation(
  dt_metadata,
  DB_cellid_header = "cell_line_identifier",
  DB_cell_annotate = c("cell_line_name", "primary_tissue", "doubling_time",
    "parental_identifier", "subtype"),
  fname = "cell_lines.csv",
  fill = "unknown",
  annotationPackage = if ("gDRinternal" %in% .packages(all.available = TRUE)) {
    "gDRinternal"
  } else {
    "gDRtestData"
  },
  externalSource = Sys.getenv("GDR_CELLLINE_ANNOTATION")
)
```

Arguments

dt_metadata	data.table with metadata
DB_cellid_header	string with colnames with cell line identifier in the annotation file
DB_cell_annotate	character vector with mandatory colnames used in the annotation file
fname	string with file name with annotation
fill	string indicating how unknown cell lines should be filled in the DB
annotationPackage	string indication name of the package containing cellline annotation
externalSource	string with path to external file with annotation data; by default it checks 'GDR_CELLLINE_ANNOTATION' env var. This file should contain columns such as gnumber, drug_name and drug_moa

Details

The logic of adding cellline annotation for dt_metadata based on the annotation file stored in gDRtestData. Other fields are set as "unknown". This approach will be corrected once we will implement final solution for adding cell lines.

Value

data.table with metadata with annotated cell lines

Examples

```
add_CellLine_annotation(  
  data.table::data.table(  
    clid = "123",  
    CellLineName = "name of the cell line")  
)
```

add_Drug_annotation *add_Drug_annotation*

Description

add drug annotation to a data.table with metadata

Usage

```
add_Drug_annotation(  
  dt_metadata,  
  fname = "drugs.csv",  
  fill = "unknown",  
  annotationPackage = if ("gDRinternal" %in% .packages(all.available = TRUE)) {  
    "gDRinternal"  
  } else {  
    "gDRtestData"  
  },  
  externalSource = Sys.getenv("GDR_DRUG_ANNOTATION")  
)
```

Arguments

dt_metadata	data.table with metadata
fname	string with file name with annotation
fill	string indicating how unknown cell lines should be filled in the DB
annotationPackage	string indication name of the package containing drug annotation
externalSource	string with path to external file with annotation data; by default it checks 'GDR_DRUG_ANNOTATION' env var. This file should contain columns such as gnumber, drug_name, and drug_moa

Details

The logic of adding drug annotation for dt_metadata based on the annotation file stored in gDRtest-Data.

Value

data.table with metadata with annotated drugs

Examples

```
add_Drug_annotation(  
  data.table::data.table(  
    Gnumber = "drug_id",  
    DrugName = "name of the drug")  
)
```

add_intermediate_data *add intermediate data (qs files) for given ma*

Description

add intermediate data (qs files) for given ma

Usage

```
add_intermediate_data(mae, data_dir, steps = get_pipeline_steps())
```

Arguments

mae	mae with dose-response data
data_dir	output directory
steps	character vector with pipeline steps for which intermediate data should be saved

Value

NULL

average_SE	<i>Run drug response processing pipeline</i>
------------	--

Description

Run different components of the gDR drug response processing pipeline. Either: create a SummarizedExperiment and normalize raw treated and control data (create_and_normalize_SE), average data (average_SE), or fit the processed data (fit_SE). See details for more in-depth explanations.

Usage

```
average_SE(  
  se,  
  data_type,  
  series_identifiers = NULL,  
  override_masked = FALSE,  
  normalized_assay = "Normalized",  
  averaged_assay = "Averaged"  
)  
  
create_SE(  
  df_,  
  data_type,  
  readout = "ReadoutValue",  
  nested_identifiers = NULL,  
  nested_confounders = intersect(names(df_), gDRutils::get_env_identifiers("barcode")),  
  override_untrt_controls = NULL  
)  
  
fit_SE(  
  se,  
  data_type = "single-agent",  
  nested_identifiers = NULL,  
  averaged_assay = "Averaged",  
  metrics_assay = "Metrics",  
  n_point_cutoff = 4,  
  range_conc = c(0.005, 5),  
  force_fit = FALSE,  
  pcutoff = 0.05,  
  cap = 0.1,  
  curve_type = c("GR", "RV")  
)  
  
normalize_SE(  
  se,  
  data_type,  
  nested_identifiers = NULL,
```

```

nested_confounders = gDRutils::get_SE_identifiers(se, "barcode", simplify = TRUE),
control_mean_fxn = function(x) {
  mean(x, trim = 0.25)
},
control_assay = "Controls",
raw_treated_assay = "RawTreated",
normalized_assay = "Normalized",
ndigit_rounding = 4
)

create_and_normalize_SE(
  df_,
  data_type,
  readout = "ReadoutValue",
  control_mean_fxn = function(x) {
    mean(x, trim = 0.25)
  },
  nested_identifiers = NULL,
  nested_confounders = intersect(names(df_), gDRutils::get_env_identifiers("barcode")),
  override_untrt_controls = NULL,
  ndigit_rounding = 4,
  control_assay = "Controls",
  raw_treated_assay = "RawTreated",
  normalized_assay = "Normalized"
)

runDrugResponseProcessingPipeline(
  x,
  readout = "ReadoutValue",
  control_mean_fxn = function(x) {
    mean(x, trim = 0.25)
  },
  nested_identifiers_l = NULL,
  nested_confounders = gDRutils::get_env_identifiers("barcode"),
  override_untrt_controls = NULL,
  override_masked = FALSE,
  ndigit_rounding = 4,
  n_point_cutoff = 4,
  control_assay = "Controls",
  raw_treated_assay = "RawTreated",
  normalized_assay = "Normalized",
  averaged_assay = "Averaged",
  metrics_assay = "Metrics",
  split_data = TRUE,
  data_dir = NULL,
  partial_run = FALSE,
  start_from = get_pipeline_steps()[1],
  selected_experiments = NULL
)

```

)

Arguments

se	SummarizedExperiment object.
data_type	single-agent vs combination
series_identifiers	character vector of identifiers in measured or metric which define a unique data point.
override_masked	boolean indicating whether or not to override the masked wells in the averaging and include all wells. Defaults to FALSE.
normalized_assay	string of the assay name containing the normalized data. Defaults to "Normalized".
averaged_assay	string of the name of the averaged assay in the SummarizedExperiment . Defaults to "Averaged".
df_	data.table of raw drug response data containing both treated and untreated values. If a column called "BackgroundValue" exists in df_, it will be removed from the readout column.
readout	string of the name containing the cell viability readout values.
nested_identifiers	character vector with the nested_identifiers for the given SE with a given data_type
nested_confounders	Character vector of the nested_confounders for a given assay. nested_keys is character vector of column names to include in the data.tables in the assays of the resulting SummarizedExperiment object. Defaults to the nested_identifiers and nested_confounders if passed through create_and_normalize_SE or runDrugResponseProcessingPipeline.
override_untrt_controls	named list containing defining factors in the treatments. Defaults to NULL.
metrics_assay	string of the name of the metrics assay to output in the returned SummarizedExperiment Defaults to "Metrics".
n_point_cutoff	integer of how many points should be considered the minimum required to try to fit a curve. Defaults to 4.
range_conc	vector of concentrations range values.
force_fit	boolean indicating whether or not to force the fit.
pcutoff	numeric cutoff value.
cap	numeric value representing the value to cap the highest allowed relative viability at.
curve_type	vector of curve type values.
control_mean_fxn	function indicating how to average controls. Defaults to mean(x, trim = 0.25).
control_assay	string containing the name of the assay representing the controls in the se. Defaults to "Controls".

raw_treated_assay	string containing the name of the assay representing the raw treated data in the se. Defaults to "RawTreated".
ndigit_rounding	integer indicating number of digits to round to in calculations. Defaults to 4.
x	data.table of MAE with drug response data
nested_identifiers_l	list with the nested_identifiers(character vectors) for single-agent and (optionally) for combination data
split_data	boolean indicating whether data provided as the MultiAssayExperiment should be split again into appropriate data types
data_dir	string with the path to the directory with intermediate data of experiments (qs files). If set to NULL (default) intermediate data is not saved/read in.
partial_run	logical flag indicating if the pipeline should be run partially (from the step defined with start_from)
start_from	string indicating the pipeline step from which partial run should be launched
selected_experiments	character vector with experiments for which pipeline should be run. This option works only for the pipeline being run partially (i.e. with partial_run flag set to TRUE)

Details

runDrugResponseProcessingPipeline is made up of 3 separate steps:

- "create_and_normalize_SE"
- "average_SE"
- "fit_SE"

For create_and_normalize_SE, this creates a SummarizedExperiment object from a data.table, where the data.table contains treatments on rows, and conditions on columns. A [SummarizedExperiment](#) object containing two assays is created: treated readouts will live in an assay called "RawTreated", and reference readouts live in an assay called "Controls". Subsequently, the treated and control elements will be normalized to output two metrics:

For average_SE, take the normalized assay and average the nested DataFrames across uniquely nested_identifiers.

For fit_SE, take the averaged assay and fit curves to obtain metrics, one set of metrics for each normalization type set.

Pipeline can be run partially with partial_run flag set to TRUE. The start_from string defines the step from which the pipeline will be launched. However, partial run of the pipeline is possible only if the whole pipeline was launched at least once with defined data_dir and intermediate data was saved as qs files into data_dir.

Pipeline can be run for the selected experiments by changing the default value of selected_experiments param. This scenario only works when partial_run is enabled.

Value

MAE object

Examples

```

d <- rep(seq(0.1, 0.9, 0.1), each = 4)
v <- rep(seq(0.1, 0.4, 0.1), 9)
df <- S4Vectors::DataFrame(
  Concentration = d,
  masked = rep(c(TRUE, TRUE, TRUE, FALSE), 9),
  normalization_type = rep(c("GR", "RV"), length(v) * 2),
  x = rep(v, 2)
)
normalized <- BumpyMatrix::splitAsBumpyMatrix(row = 1, column = 1, x = df)

keys <- list(Trt = "Concentration", "masked_tag" = "masked")
assays <- list("Normalized" = normalized)
se <- SummarizedExperiment::SummarizedExperiment(assays = assays)
se <- gDRutils::set_SE_keys(se, keys)
se <- gDRutils::set_SE_identifiers(se, gDRutils::get_env_identifiers())
se1 <- average_SE(
  se,
  data_type = "single-agent",
  override_masked = FALSE,
  normalized_assay = "Normalized",
  averaged_assay = "Averaged"
)

td <- gDRimport::get_test_data()
l_tbl <- gDRimport::load_data(
  manifest_file = gDRimport::manifest_path(td),
  df_template_files = gDRimport::template_path(td),
  results_file = gDRimport::result_path(td)
)
imported_data <- merge_data(
  l_tbl$manifest,
  l_tbl$treatments,
  l_tbl$data
)

se <- purrr::quietly(create_SE)(imported_data, data_type = "single-agent")

td <- gDRimport::get_test_data()
l_tbl <- gDRimport::load_data(
  manifest_file = gDRimport::manifest_path(td),
  df_template_files = gDRimport::template_path(td),
  results_file = gDRimport::result_path(td)
)
imported_data <- merge_data(
  l_tbl$manifest,
  l_tbl$treatments,
  l_tbl$data
)

```

```

inl <- prepare_input(imported_data)
se <- create_SE(
  inl$df_list[["single-agent"]],
  data_type = "single-agent",
  nested_confounders = inl$nested_confounders)

normalize_SE(se, data_type = "single-agent")
p_dir <- file.path(tempdir(), "pcheck")
dir.create(p_dir)
td <- gDRimport::get_test_data()
l_tbl <- gDRimport::load_data(
  manifest_file = gDRimport::manifest_path(td),
  df_template_files = gDRimport::template_path(td),
  results_file = gDRimport::result_path(td)
)
imported_data <- merge_data(
  l_tbl$manifest,
  l_tbl$treatments,
  l_tbl$data
)
runDrugResponseProcessingPipeline(
  imported_data,
  data_dir = p_dir
)

```

calculate_excess

Calculate the difference between values in two data.tables

Description

Calculate the difference between values, likely representing the same metric, from two data.tables.

Usage

```

calculate_excess(
  metric,
  measured,
  series_identifiers,
  metric_col,
  measured_col
)

```

Arguments

metric	data.table often representing readouts derived by calculating some metric. Examples of this could include hsa or bliss calculations from single-agent data.
measured	data.table often representing measured data from an experiment.

series_identifiers character vector of identifiers in measured or metric which define a unique data point.
metric_col string of the column in metric to use in excess calculation.
measured_col string of the column in measured to use in excess calculation.

Value

data.table of measured, now with an additional column named excess (positive values for synergy/benefit).

Examples

```

metric <- data.table::data.table(
  Concentration = c(1, 2, 3, 1, 2, 3),
  Concentration_2 = c(1, 1, 1, 2, 2, 2),
  GRvalue = c(100, 200, 300, 400, 500, 600)
)
measured <- data.table::data.table(
  Concentration = c(3, 1, 2, 2, 1, 3),
  Concentration_2 = c(1, 1, 1, 2, 2, 2),
  testvalue = c(200, 0, 100, 400, 300, 500)
)
series_identifiers <- c("Concentration", "Concentration_2")
metric_col <- "GRvalue"
measured_col <- "testvalue"
calculate_excess(
  metric,
  measured,
  series_identifiers,
  metric_col,
  measured_col
)

```

calculate_GR_value *Calculate a GR value.*

Description

Calculate a GR value for a given set of dose response values.

Usage

```

calculate_GR_value(
  rel_viability,
  corrected_readout,
  day0_readout,
  untrt_readout,

```

```

    ndigit_rounding,
    duration,
    ref_div_time,
    cap = 1.25
)

calculate_time_dep_GR_value(
  corrected_readout,
  day0_readout,
  untrt_readout,
  ndigit_rounding
)

calculate_endpt_GR_value(
  rel_viability,
  duration,
  ref_div_time,
  cap = 1.25,
  ndigit_rounding
)

```

Arguments

<code>rel_viability</code>	numeric vector representing the Relative Viability.
<code>corrected_readout</code>	numeric vector containing the corrected readout.
<code>day0_readout</code>	numeric vector containing the day 0 readout.
<code>untrt_readout</code>	numeric vector containing the untreated readout.
<code>ndigit_rounding</code>	integer specifying the number of digits to use for calculation rounding.
<code>duration</code>	numeric value specifying the length of time the cells were treated (in hours).
<code>ref_div_time</code>	numeric value specifying the reference division time for the cell line in the experiment.
<code>cap</code>	numeric value representing the value to cap the highest allowed relative viability at.

Details

Note that this function expects that all numeric vectors are of the same length. `calculate_GR_value` will try to greedily calculate a GR value. If no day 0 readouts are available, the `duration` and `ref_div_time` will be used to try to back-calculate a day 0 value in order to produce a GR value.

In the case of calculating the reference GR value from multiple reference readout values, the vectorized calculation is performed and then the resulting vector should be averaged outside of this function.

Note that it is expected that the `ref_div_time` and `duration` are reported in the same units.

Value

numeric vector containing GR values, one value for each element of the input vectors.

See Also

normalize_SE2

Examples

```
duration <- 144
rv <- seq(0.1, 1, 0.1)
corrected <- seq(41000, 50000, 1000)
day0 <- seq(91000, 95500, 500)
untrt <- rep(c(115000, 118000), 5)

calculate_GR_value(
  rel_viability = rv,
  corrected_readout = corrected,
  day0_readout = day0,
  untrt_readout = untrt,
  ndigit_rounding = 4,
  duration = duration,
  ref_div_time = duration / 2
)

readouts <- rep(10000, 5)
calculate_time_dep_GR_value(readouts, readouts * 1.32, readouts * 2, 2)

readouts <- rep(10000, 5)
calculate_endpt_GR_value(readouts, 72, 1, ndigit_rounding = 2)
```

calculate_matrix_metric

Calculate a metric for combination data.

Description

Calculate a metric based off of single-agent values in combination screens.

Usage

```
calculate_HSA(sa1, series_id1, sa2, series_id2, metric)

calculate_Bliss(
  sa1,
  series_id1,
  sa2,
  series_id2,
```

```

    metric,
    measured_col = "smooth"
  )

  .calculate_matrix_metric(
    sa1,
    series_id1,
    sa2,
    series_id2,
    metric,
    FXN,
    measured_col = "x"
  )

```

Arguments

sa1	data.table containing single agent data where entries in series_id2 are all 0. Columns of the data.table include identifiers and the metric of interest. Metric is stored in the 'x' column.
series_id1	String representing the column within sa1 that represents id1.
sa2	data.table containing single agent data where entries in series_id1 are all 0. Columns of the data.table include identifiers and the metric of interest. Metric is stored in the 'x' column.
series_id2	String representing the column within sa2 that represents id2.
metric	String specifying the metric of interest. Usually either 'GRvalue' or 'Relative-Viability'.
measured_col	String specifying the measured colname.
FXN	Function to apply to the single-agent fits to calculate a metric.

Details

calculate_HSA takes the minimum of the two single agents readouts. calculate_Bliss performs Bliss additivity calculation based on the single agent effects, defined as $1-x$ for the corresponding normalization. See <https://www.sciencedirect.com/science/article/pii/S1359644619303460?via%3Dihub#tb0005> for more details.

Value

data.table containing a single row for every unique combination of the two series identifiers and the corresponding calculated metric for each row.

Examples

```

n <- 10
sa1 <- data.table::data.table(conc = seq(n), conc2 = rep(0, n), smooth = seq(n))
sa2 <- data.table::data.table(conc = rep(0, n), conc2 = seq(n), smooth = seq(n))
calculate_HSA(sa1, "conc", sa2, "conc2", "smooth")
n <- 10

```

```
sa1 <- data.table::data.table(conc = seq(n), conc2 = rep(0, n), smooth = seq(n))
sa2 <- data.table::data.table(conc = rep(0, n), conc2 = seq(n), smooth = seq(n))
calculate_Bliss(sa1, "conc", sa2, "conc2", "smooth")
```

cleanup_metadata	<i>cleanup_metadata</i>
------------------	-------------------------

Description

Cleanup a data.table with metadata

Usage

```
cleanup_metadata(df_metadata)
```

Arguments

df_metadata a data.table with metadata

Details

Adds annotations and check whether user provided correct input data.

Value

a data.table with cleaned metadata

Examples

```
df <- data.table::data.table(
  clid = "CELL_LINE",
  Gnumber = "DRUG_1",
  Concentration = c(0, 1),
  Duration = 72
)
cleanup_df <- cleanup_metadata(df)
```

`convert_mae_to_raw_data`*Transform mae into raw data*

Description

Transform mae into raw data

Usage

```
convert_mae_to_raw_data(mae)
```

Arguments

`mae` MultiAssayExperiment object with SummarizedExperiments containing "RawTreated" and "Controls" assays

Value

data.table with raw data

Examples

```
mae <- gDRutils::get_synthetic_data("finalMAE_small")
convert_mae_to_raw_data(mae)
```

`convert_se_to_raw_data`*Transform se into raw_data*

Description

Transform se into raw_data

Usage

```
convert_se_to_raw_data(se)
```

Arguments

`se` SummarizedExperiment object with "RawTreated" and "Controls" assays

Value

data.table with raw data

Examples

```
mae <- gDRutils::get_synthetic_data("finalMAE_small")
se <- mae[[1]]
convert_se_to_raw_data(se)
```

data_model	<i>Detect model of data</i>
------------	-----------------------------

Description

Detect model of data

Usage

```
data_model(x)
```

Arguments

x data.table with raw data or SummarizedExperiment object with gDR assays

Value

string with the information of the raw data follows single-agent or combination data model

Examples

```
data_model("single-agent")
```

data_model.character	<i>Detect model of data from experiment name</i>
----------------------	--

Description

Detect model of data from experiment name

Usage

```
## S3 method for class 'character'
data_model(x)
```

Arguments

x character with experiment name

Value

string with the information of the raw data follows single-agent or combination data model

data_model.data.table *Detect model of data in data.table*

Description

Detect model of data in data.table

Usage

```
## S3 method for class 'data.table'  
data_model(x)
```

Arguments

x data.table of raw drug response data containing both treated and untreated values.

Value

string with the information of the raw data follows single-agent or combination data model

define_matrix_grid_positions
Define matrix grid positions

Description

Define matrix grid positions

Usage

```
define_matrix_grid_positions(conc1, conc2)
```

Arguments

conc1 drug_1 concentration
conc2 drug_2 concentration

Details

drug_1 is diluted along the rows as the y-axis and drug_2 is diluted along the columns and will be the x-axis.

Value

list with axis grid positions

do_skip_step	<i>check if the given step can be skipped if partial run is chosen</i>
--------------	--

Description

check if the given step can be skipped if partial run is chosen

Usage

```
do_skip_step(current_step, start_from, steps = get_pipeline_steps())
```

Arguments

current_step	string with the step to be evaluated
start_from	string indicating the pipeline step from which partial run should be launched
steps	charvect with all available steps

Value

logical

fit_SE.combinations	<i>fit_SE for combination screens</i>
---------------------	---------------------------------------

Description

Perform fittings for combination screens.

Usage

```
fit_SE.combinations(  
  se,  
  data_type = gDRutils::get_experiment_groups("combination"),  
  series_identifiers = NULL,  
  normalization_types = c("GR", "RV"),  
  averaged_assay = "Averaged",  
  metrics_assay = "Metrics"  
)
```

Arguments

se	SummarizedExperiment object with a BumpyMatrix assay containing averaged data.
data_type	single-agent vs combination
series_identifiers	character vector of the column names in the nested DFrame corresponding to nested identifiers.
normalization_types	character vector of normalization types used for calculating combo matrix.
averaged_assay	string of the name of the averaged assay to use as input. in the se.
metrics_assay	string of the name of the metrics assay to output in the returned SummarizedExperiment . whose combination represents a unique series for which to fit curves.

Details

This function assumes that the combination is set up with both concentrations nested in the assay.

Value

A SummarizedExperiment object with an additional assay containing the combination metrics.

Examples

```
fmae_cms <- gDRutils::get_synthetic_data("finalMAE_combo_matrix_small")

se1 <- fmae_cms[[gDRutils::get_experiment_groups("combination")]]
SummarizedExperiment::assays(se1) <-
  SummarizedExperiment::assays(se1)["Averaged"]
fit_SE.combinations(se1[1, 1])
```

generateCodilution *generateCodilution*

Description

generateCodilution

Usage

```
generateCodilution(cell_lines, drugs, save = TRUE)
```

Value

data.table with raw input data or MAE with processed data

`generateCodilutionSmall`
generateCodilutionSmall

Description

`generateCodilutionSmall`

Usage

`generateCodilutionSmall(cell_lines, drugs, save = TRUE)`

Value

data.table with raw input data or MAE with processed data

`generateComboMatrix` *generateComboMatrix*

Description

`generateComboMatrix`

Usage

`generateComboMatrix(cell_lines, drugs, save = TRUE)`

Value

data.table with raw input data or MAE with processed data

`generateComboMatrixSmall`
generateComboMatrixSmall

Description

`generateComboMatrixSmall`

Usage

`generateComboMatrixSmall(cell_lines, drugs, save = TRUE)`

Value

data.table with raw input data or MAE with processed data

`generateComboNoNoiseData`
generateComboNoNoiseData

Description

`generateComboNoNoiseData`

Usage

```
generateComboNoNoiseData(cell_lines, drugs, save = TRUE)
```

Value

data.table with raw input data or MAE with processed data

`generateComboNoNoiseData2`
generateComboNoNoiseData2

Description

`generateComboNoNoiseData2`

Usage

```
generateComboNoNoiseData2(cell_lines, drugs, save = TRUE)
```

Value

data.table with raw input data or MAE with processed data

`generateComboNoNoiseData3`
generateComboNoNoiseData3

Description

`generateComboNoNoiseData3`

Usage

```
generateComboNoNoiseData3(cell_lines, drugs, save = TRUE)
```

Value

data.table with raw input data or MAE with processed data

`generateLigandData` *generateLigandData*

Description

`generateLigandData`

Usage

`generateLigandData(cell_lines, drugs, save = TRUE)`

Value

data.table with raw input data or MAE with processed data

`generateMediumData` *generateMediumData*

Description

`generateMediumData`

Usage

`generateMediumData(cell_lines, drugs, save = TRUE)`

Value

data.table with raw input data or MAE with processed data

`generateNoiseRawData` *generateNoiseRawData*

Description

`generateNoiseRawData`

Usage

`generateNoiseRawData(cell_lines, drugs, save = TRUE)`

Value

data.table with raw input data or MAE with processed data

`generateNoNoiseRawData`

generateNoNoiseRawData

Description

`generateNoNoiseRawData`

Usage

`generateNoNoiseRawData(cell_lines, drugs, save = TRUE)`

Value

data.table with raw input data or MAE with processed data

`generateTripleComboMatrix`

generateTripleComboMatrix

Description

`generateTripleComboMatrix`

Usage

`generateTripleComboMatrix(cell_lines, drugs, save = TRUE)`

Value

data.table with raw input data or MAE with processed data

get_assays_per_pipeline_step
get info about created/present assays in SE at the given pipeline step

Description

get info about created/present assays in SE at the given pipeline step

Usage

```
get_assays_per_pipeline_step(  
  step,  
  data_model,  
  status = c("created", "present")  
)
```

Arguments

step	string with pipeline step
data_model	single-agent vs combination
status	string return vector of assays created or present at the given step?

Value

assay

get_default_nested_identifiers
Get default nested identifiers

Description

Get default nested identifiers

Usage

```
get_default_nested_identifiers(x, data_model = NULL)  
  
## S3 method for class 'data.table'  
get_default_nested_identifiers(x, data_model = NULL)  
  
## S3 method for class 'SummarizedExperiment'  
get_default_nested_identifiers(x, data_model = NULL)
```

Arguments

`x` data.table with raw data or SummarizedExperiment object with gDR assays
`data_model` single-agent vs combination

Value

vector of nested identifiers

Examples

```
get_default_nested_identifiers(data.table::data.table())
```

```
get_mae_from_intermediate_data
      get mae dataset from intermediate data
```

Description

get mae dataset from intermediate data

Usage

```
get_mae_from_intermediate_data(data_dir)
```

Arguments

`data_dir` directory with intermediate data

Value

MAE object

```
get_pipeline_steps      get pipeline steps
```

Description

get pipeline steps

Usage

```
get_pipeline_steps()
```

Value

vector with steps

grr_matches	<i>Value Matching</i>
-------------	-----------------------

Description

Returns a lookup table or list of the positions of ALL matches of its first argument in its second and vice versa. Similar to [match](#), though that function only returns the first match.

Usage

```
grr_matches(
  x,
  y,
  all.x = TRUE,
  all.y = TRUE,
  list = FALSE,
  indexes = TRUE,
  nomatch = NA
)
```

Arguments

x	vector. The values to be matched. Long vectors are not currently supported.
y	vector. The values to be matched. Long vectors are not currently supported.
all.x	logical; if TRUE, then each value in x will be included even if it has no matching values in y
all.y	logical; if TRUE, then each value in y will be included even if it has no matching values in x
list	logical. If TRUE, the result will be returned as a list of vectors, each vector being the matching values in y. If FALSE, result is returned as a data.table with repeated values for each match.
indexes	logical. Whether to return the indices of the matches or the actual values.
nomatch	the value to be returned in the case when no match is found. If not provided and indexes=TRUE, items with no match will be represented as NA. If set to NULL, items with no match will be set to an index value of length+1. If indexes=FALSE, they will default to NA.

Details

This behavior can be imitated by using joins to create lookup tables, but `matches` is simpler and faster: usually faster than the best joins in other packages and thousands of times faster than the built in [merge](#).

`all.x/all.y` correspond to the four types of database joins in the following way:

left `all.x=TRUE, all.y=FALSE`

right all.x=FALSE, all.y=TRUE

inner all.x=FALSE, all.y=FALSE

full all.x=TRUE, all.y=TRUE

Note that NA values will match other NA values.

Source of the function: <https://github.com/cran/grr/blob/master/R/grr.R>

Value

data.table

Examples

```
mat_elem <- data.table::data.table(
  DrugName = rep(c("untreated", "drugA", "drugB", "untreated"), 2),
  DrugName_2 = rep(c("untreated", "vehicle", "drugA", "drugB"), 2),
  clid = rep(c("C1", "C2"), each = 4)
)
untreated_tag <- gDRutils::get_env_identifiers("untreated_tag")
ref_idx <- which(
  mat_elem$DrugName %in% untreated_tag |
  mat_elem$DrugName_2 %in% untreated_tag
)
ref <- mat_elem[ref_idx, ]
treated <- mat_elem[-ref_idx, ]
valid <- c("DrugName", "DrugName_2")
trt <- lapply(valid, function(x) {
  colnames <- c("clid", x)
  treated[, colnames, with = FALSE]
})
trt <- do.call(paste,
  do.call(rbind, lapply(trt, function(x) setNames(x, names(trt[[1]]))))
)
ref <- lapply(valid, function(x) {
  colnames <- c("clid", x)
  ref[, colnames, with = FALSE]
})
ref <- do.call(paste,
  do.call(rbind, lapply(ref, function(x) setNames(x, names(ref[[1]]))))
)
grr_matches(trt, ref, list = FALSE, all.y = FALSE)
```

identify_data_type *Identify type of data*

Description

Identify type of data

Usage

```
identify_data_type(df, codilution_conc = 2, matrix_conc = 1)
```

Arguments

<code>df</code>	data.table of raw drug response data containing both treated and untreated values
<code>codilution_conc</code>	integer of maximum number of concentration ratio of co-treatment to classify as codilution data type; defaults to 2
<code>matrix_conc</code>	integer of minimum number of concentration pairs of co-treatment to classify as co-treatment or matrix data type; defaults to 1

Value

data.table of raw drug response data with additional column `type` with the info of data type for a given row of data.table

Author(s)

Bartosz Czech bartosz.czech@contractors.roche.com

Examples

```
conc <- rep(seq(0, 0.3, 0.1), 2)
ctrl_df <- S4Vectors::DataFrame(
  ReadoutValue = c(2, 2, 1, 1, 2, 1),
  Concentration = rep(0, 6),
  masked = FALSE,
  DrugName = rep(c("DRUG_10", "vehicle", "DRUG_8"), 2),
  CellLineName = "CELL1"
)

trt_df <- S4Vectors::DataFrame(
  ReadoutValue = rep(seq(1, 4, 1), 2),
  Concentration = conc,
  masked = rep(FALSE, 8),
  DrugName = c("DRUG_10", "DRUG_8"),
  CellLineName = "CELL1"
)
input_df <- data.table::as.data.table(rbind(ctrl_df, trt_df))
input_df$Duration <- 72
input_df$CorrectedReadout2 <- input_df$ReadoutValue
identify_data_type(input_df)
```

identify_keys	<i>identify_keys</i>
---------------	----------------------

Description

Group columns from a `data.table` that correspond to different

Usage

```
identify_keys(
  df_,
  nested_keys = NULL,
  override_untrt_controls = NULL,
  identifiers = gDRutils::get_env_identifiers()
)
```

Arguments

`df_` a `data.table` to identify keys for.

`nested_keys` character vector of keys to exclude from the returned list. The keys discarded should be identical to the keys in the third dimension of the `SummarizedExperiment`. Defaults to the "Barcode" and the masked identifier.

`override_untrt_controls` named list containing defining factors in the treatments. Defaults to `NULL`.

`identifiers` named list containing all identifiers to use during processing. By default, this value will be obtained by the environment.

Details

This is most likely to be used for provenance tracking and will be placed on the `SummarizedExperiment` metadata for downstream analyses to reference.

Value

named list of key types and their corresponding key values.

See Also

`map_df`, `create_SE`

Examples

```
n <- 64
md_df <- data.table::data.table(
  Gnumber = rep(c("vehicle", "untreated", paste0("G", seq(2))), each = 16),
  DrugName = rep(c("vehicle", "untreated", paste0("GN", seq(2))), each = 16),
  clid = paste0("C", rep_len(seq(4), n)),
  CellLineName = paste0("N", rep_len(seq(4), n)),
```

```

replicates = rep_len(paste0("R", rep(seq(4), each = 4)), 64),
drug_moa = "inhibitor",
ReferenceDivisionTime = rep_len(c(120, 60), n),
Tissue = "Lung",
parental_identififier = "CL12345",
Duration = 160
)
md_df <- unique(md_df)
ref <- md_df$Gnumber %in% c("vehicle", "untreated")
trt_df <- md_df[!ref, ]
identify_keys(trt_df)

```

is_preceding_step	<i>check if the given step is preceding the step chosen in the partial run</i>
-------------------	--

Description

check if the given step is preceding the step chosen in the partial run

Usage

```
is_preceding_step(current_step, start_from, steps = get_pipeline_steps())
```

Arguments

current_step	string with the step to be evaluated
start_from	string indicating the pipeline step from which partial run should be launched
steps	charvect with all available steps

Value

logical

map_conc_to_standardized_conc	<i>Create a mapping of concentrations to standardized concentrations.</i>
-------------------------------	---

Description

Create a mapping of concentrations to standardized concentrations.

Usage

```
map_conc_to_standardized_conc(conc1, conc2)
```

Arguments

conc1 numeric vector of the concentrations for drug 1.
 conc2 numeric vector of the concentrations for drug 2.

Details

The concentrations are standardized in that they will contain regularly spaced dilutions and close values will be rounded.

Value

data.table of 2 columns named "concs" and "rconcs" containing the original concentrations and their closest matched standardized concentrations respectively. and their new standardized concentrations.

See Also

replace_conc_w_standardized_conc

Examples

```
ratio <- 0.5
conc1 <- c(0, 10 ^ (seq(-3, 1, ratio)))

shorter_range <- conc1[-1]
noise <- runif(length(shorter_range), 1e-12, 1e-11)
conc2 <- shorter_range + noise

map_conc_to_standardized_conc(conc1, conc2)
```

 map_df

Map treated conditions to their respective references.

Description

Map treated conditions to their respective Day0, untreated, or single-agent references using condition metadata.

Usage

```
map_df(
  trt_md,
  ref_md,
  override_untrt_controls = NULL,
  ref_cols,
  ref_type = c("Day0", "untrt_Endpoint")
)
```

Arguments

trt_md	data.table of treated metadata.
ref_md	data.table of untreated metadata.
override_untrt_controls	named list indicating what treatment metadata fields should be used as a control. Defaults to NULL.
ref_cols	character vector of the names of reference columns to include. Likely obtained from identify_keys().
ref_type	string of the reference type to map to. Should be one of c("Day0", "untrt_Endpoint", "ref_Endpoint").

Details

If override_untrt_controls is specified, TODO: FILL ME!

Value

named list mapping treated metadata to untreated metadata.

See Also

identify_keys

Examples

```
n <- 64
md_df <- data.table::data.table(
  Gnumber = rep(c("vehicle", "untreated", paste0("G", seq(2))), each = 16),
  DrugName = rep(c("vehicle", "untreated", paste0("GN", seq(2))), each = 16),
  clid = paste0("C", rep_len(seq(4), n)),
  CellLineName = paste0("N", rep_len(seq(4), n)),
  replicates = rep_len(paste0("R", rep(seq(4), each = 4)), 64),
  drug_moa = "inhibitor",
  ReferenceDivisionTime = rep_len(c(120, 60), n),
  Tissue = "Lung",
  parental_identifier = "CL12345",
  Duration = 160
)
md_df <- unique(md_df)
ref <- md_df$Gnumber %in% c("vehicle", "untreated")
ref_df <- md_df[ref, ]
trt_df <- md_df[!ref, ]
Keys <- identify_keys(trt_df)
ref_type <- "untrt_Endpoint"
map_df(
  trt_df,
  ref_df,
  ref_cols = Keys[[ref_type]],
  ref_type = ref_type
)
```

map_ids_to_fits	<i>Get predicted values for a given fit and input.</i>
-----------------	--

Description

Map fittings to identifiers and compute the predicted values for corresponding fits.

Usage

```
map_ids_to_fits(pred, match_col, fittings, fitting_id_col)
```

Arguments

pred	numeric vector for which you want predictions.
match_col	vector to match on fittings to get the correct fit.
fittings	data.table of fit metrics.
fitting_id_col	string of the column name in fittings that should be used to match with match_col.

Value

Numeric vector of predicted values given pred inputs and fittings values.

Examples

```
pred <- c(1, 5, 5)
match_col <- c(1, 1, 2)
fitting_id_col <- "match_on_me"

fit1 <- data.table::data.table(h = 2.09, x_inf = 0.68, x_0 = 1, ec50 = 0.003)
fit2 <- data.table::data.table(h = 0.906, x_inf = 0.46, x_0 = 1, ec50 = 0.001)
fittings <- do.call(rbind, list(fit1, fit2))
fittings[[fitting_id_col]] <- c(1, 2)

map_ids_to_fits(pred, match_col, fittings, fitting_id_col)
```

map_untreated	<i>Identify untreated rows based on Drug treatment alone</i>
---------------	--

Description

Identify untreated rows based on Drug treatment alone

Usage

```
map_untreated(mat_elem)
```

Arguments

mat_elem	input data frame
----------	------------------

Details

Using the given rownames, map the untreated conditions

Value

list

merge_data	<i>merge_data</i>
------------	-------------------

Description

Merge all the input data into a single data.table

Usage

```
merge_data(manifest, treatments, data)
```

Arguments

manifest	a data.table with a manifest info
treatments	a data.table with a treatatments info
data	a data.table with a raw data info

Value

a data.table with merged data and metadata.

Examples

```
td <- gDRimport::get_test_data()
l_tbl <- gDRimport::load_data(
  manifest_file = gDRimport::manifest_path(td),
  df_template_files = gDRimport::template_path(td),
  results_file = gDRimport::result_path(td)
)
merge_data(
  l_tbl$manifest,
  l_tbl$treatments,
  l_tbl$data
)
```

order_result_df	<i>Order_result_df</i>
-----------------	------------------------

Description

Order a data.table with results

Usage

```
order_result_df(df_)
```

Arguments

df_ a data.table with results

Value

a ordered data.table with results

prepare_input	<i>Prepare input data common for all experiments</i>
---------------	--

Description

Current steps

- refining nested confounders
- refining nested identifiers
- splitting df_ into (per experiment) df_list

Usage

```
prepare_input(x, ...)
```


Arguments

x data.table with raw data or MAE object with dose-reponse data
... additional parameters

Value

list of input data

Examples

```
td <- gDRimport::get_test_data()
l_tbl <- gDRimport::load_data(
  manifest_file = gDRimport::manifest_path(td),
  df_template_files = gDRimport::template_path(td),
  results_file = gDRimport::result_path(td)
)
df_ <- merge_data(
  l_tbl$manifest,
  l_tbl$treatments,
  l_tbl$data
)
nested_confounders = intersect(
  names(df_),
  gDRutils::get_env_identifiers("barcode")
)
prepare_input(df_, nested_confounders, NULL)
```

prepare_input.data.table

Prepare input data common for all experiments

Description

Current steps

- refining nested confounders
- refining nested identifiers
- splitting df_ into (per experiment) df_list

Usage

```
## S3 method for class 'data.table'
prepare_input(
  x,
  nested_confounders = gDRutils::get_env_identifiers("barcode"),
  nested_identifiers_l = .get_default_nested_identifiers(),
  ...
)
```

Arguments

x data.table with raw data
nested_confounders Character vector of the nested_confounders for a given assay. **nested_keys** is character vector of column names to include in the data.tables in the assays of the resulting SummarizedExperiment object. Defaults to the **nested_identifiers** and **nested_confounders** if passed through
nested_identifiers_l list with the nested_identifiers(character vectors) for single-agent and (optionally) for combination data
... additional parameters

Value

list of input data

```
prepare_input.MultiAssayExperiment
```

Prepare input data common for all experiments

Description

Current steps

- refining nested confounders
- refining nested identifiers
- splitting df_ into (per experiment) df_list

Usage

```
## S3 method for class 'MultiAssayExperiment'
prepare_input(
  x,
  nested_confounders = gDRutils::get_SE_identifiers(x[[1]], "barcode"),
  nested_identifiers_l = .get_default_nested_identifiers(x[[1]]),
  raw_data_field = "experiment_raw_data",
  split_data = TRUE,
  ...
)
```

Arguments

x	MAE object with dose-reponse data
nested_confounders	Character vector of the nested_confounders for a given assay. nested_keys is character vector of column names to include in the data.tables in the assays of the resulting SummarizedExperiment object. Defaults to the nested_identifiers and nested_confounders if passed through
nested_identifiers_l	list with the nested_identifiers(character vectors) for single-agent and (optionally) for combination data
raw_data_field	metadata field with raw data
split_data	Boolean indicating need of splitting the data into experiment types
...	additional parameters

Value

list of input data

read_intermediate_data

read intermediate data for the given experiment and step to qs file

Description

read intermediate data for the given experiment and step to qs file

Usage

```
read_intermediate_data(path, step, experiment)
```

Arguments

path	string with the input directory of the qs file
step	string with the step name
experiment	string with the experiment name

Value

se

remove_drug_batch *Remove batch from Gnumber*

Description

Remove batch from Gnumber

Usage

```
remove_drug_batch(drug)
```

Arguments

drug drug name

Value

Gnumber without a batch

Examples

```
remove_drug_batch("DRUG.123")
```

replace_conc_with_standardized_conc
Standardize concentrations.

Description

Utilize a map to standardize concentrations.

Usage

```
replace_conc_with_standardized_conc(  
  original_concs,  
  conc_map,  
  original_conc_col,  
  standardized_conc_col  
)
```

Arguments

`original_concs` numeric vector of concentrations to replace using `conc_map`.
`conc_map` data.table of two columns named `original_conc_col` and `standardized_conc_col`.
`original_conc_col` string of the name of the column in `conc_map` containing the original concentrations to replace.
`standardized_conc_col` string of the name of the column in `conc_map` containing the standardized concentrations to use for replacement.

Value

numeric vector of standardized concentrations.

See Also

`map_conc_to_standardized_conc`

Examples

```
conc_map <- data.table::data.table(  
  orig = c(0.99, 0.6, 0.456, 0.4),  
  std = c(1, 0.6, 0.46, 0.4)  
)  
original_concs <- c(0.456, 0.456, 0.4, 0.99)  
exp <- c(0.46, 0.46, 0.4, 1)  
obs <- replace_conc_with_standardized_conc(  
  original_concs,  
  conc_map,  
  original_conc_col = "orig",  
  standardized_conc_col = "std"  
)
```

`round_concentration` *Round concentration to ndigit significant digits*

Description

Round concentration to ndigit significant digits

Usage

```
round_concentration(x, ndigit = 3)
```

Arguments

`x` value to be rounded.
`ndigit` number of significant digits (default = 4).

Value

rounded x

Examples

```
round_concentration(x = c(0.00175,0.00324,0.0091), ndigit = 1)
```

save_intermediate_data

save intermediate data for the given experiment and step to qs file

Description

save intermediate data for the given experiment and step to qs file

Usage

```
save_intermediate_data(path, step, experiment, se)
```

Arguments

path	string with the save directory for the qs file
step	string with the step name
experiment	string with the experiment name
se	output se

Value

NULL

split_raw_data

Split raw data into list based on the data types

Description

Split raw data into list based on the data types

Usage

```
split_raw_data(df, type_col = "type")
```

Arguments

`df` data.table of raw drug response data containing both treated and untreated values with column specified in `type_col` argument.

`type_col` string with column names in `df` with info about data type. Defaults to "type".

Value

list with split data based on its data type

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Examples

```
cell_lines <- gDRtestData::create_synthetic_cell_lines()
drugs <- gDRtestData::create_synthetic_drugs()
df_layout <- drugs[4:6, as.list(cell_lines[7:8, ]), names(drugs)]
df_layout <- gDRtestData::add_data_replicates(df_layout)
df_layout <- gDRtestData::add_concentration(
  df_layout,
  concentrations = 10 ^ (seq(-3, .5, .5))
)

df_2 <-
  drugs[c(21, 26), as.list(cell_lines[which(cell_lines$clid %in% df_layout$clid)]), names(drugs)]
df_2 <- gDRtestData::add_data_replicates(df_2)
df_2 <- gDRtestData::add_concentration(
  df_2,
  concentrations = 10 ^ (seq(-3, .5, .5))
)
colnames(df_2)[colnames(df_2) %in% c(colnames(drugs), "Concentration")] <-
  paste0(
    colnames(df_2)[colnames(df_2) %in% c(colnames(drugs), "Concentration")],
    "_2"
  )
df_layout_2 <- df_layout[df_2, on = intersect(names(df_layout), names(df_2)),
  allow.cartesian = TRUE]
df_merged_data <- gDRtestData::generate_response_data(df_layout_2, 0)
df <- identify_data_type(df_merged_data)
split_raw_data(df)

conc <- rep(seq(0, 0.3, 0.1), 2)
ctrl_df <- S4Vectors::DataFrame(
  ReadoutValue = c(2, 2, 1, 1, 2, 1),
  Concentration = rep(0, 6),
  masked = FALSE,
  DrugName = rep(c("DRUG_10", "vehicle", "DRUG_8"), 2),
  CellLineName = "CELL1"
)
```

```

trt_df <- S4Vectors::DataFrame(
  ReadoutValue = rep(seq(1, 4, 1), 2),
  Concentration = conc,
  masked = rep(FALSE, 8),
  DrugName = c("DRUG_10", "DRUG_8"),
  CellLineName = "CELL1"
)
input_df <- data.table::as.data.table(rbind(ctrl_df, trt_df))
input_df$Duration <- 72
input_df$CorrectedReadout2 <- input_df$ReadoutValue
split_df <- identify_data_type(input_df)
split_raw_data(split_df)

```

test_synthetic_data *Testing synthetic data form gDRtestData package*

Description

Testing synthetic data form gDRtestData package

Usage

```

test_synthetic_data(
  original,
  data,
  dataName,
  override_untrt_controls = NULL,
  assays = c("Normalized", "Averaged", "Metrics"),
  tolerance = 0.001
)

```

Arguments

original	original MAE assay
data	datase MAE or data.table
dataName	dataset name
override_untrt_controls	named list containing defining factors in the treatments
assays	assays to test
tolerance	tolerance factor

Value

NULL

Examples

```
set.seed(2)
cell_lines <- gDRtestData::create_synthetic_cell_lines()
drugs <- gDRtestData::create_synthetic_drugs()
data <- "finalMAE_small"
original <- gDRutils::get_synthetic_data(data)
test_synthetic_data(original, original, "test")
```

Index

- * **annotation**
 - add_CellLine_annotation, 6
 - add_Drug_annotation, 7
 - remove_drug_batch, 44
- * **calculate_GR**
 - calculate_GR_value, 15
- * **combinations**
 - calculate_excess, 14
 - calculate_matrix_metric, 17
 - define_matrix_grid_positions, 22
- * **convert_to_raw_data**
 - convert_mae_to_raw_data, 20
 - convert_se_to_raw_data, 20
- * **data_type**
 - identify_data_type, 32
 - split_raw_data, 46
- * **internal**
 - add_intermediate_data, 8
 - do_skip_step, 23
 - gDRcore-package, 3
 - generateCodilution, 24
 - generateCodilutionSmall, 25
 - generateComboMatrix, 25
 - generateComboMatrixSmall, 25
 - generateComboNoNoiseData, 26
 - generateComboNoNoiseData2, 26
 - generateComboNoNoiseData3, 26
 - generateLigandData, 27
 - generateMediumData, 27
 - generateNoiseRawData, 27
 - generateNoNoiseRawData, 28
 - generateTripleComboMatrix, 28
 - get_mae_from_intermediate_data, 30
 - get_pipeline_steps, 30
 - is_preceding_step, 35
 - read_intermediate_data, 43
 - save_intermediate_data, 46
- * **map_df**
 - .map_references, 4
 - map_df, 36
 - map_ids_to_fits, 38
 - map_untreated, 39
- * **merge_data**
 - merge_data, 39
- * **prepare_input**
 - prepare_input, 40
 - prepare_input.data.table, 41
 - prepare_input.MultiAssayExperiment, 42
- * **runDrugResponseProcessingPipeline**
 - average_SE, 9
 - fit_SE.combinations, 23
- * **test_utils**
 - test_synthetic_data, 48
- * **utils**
 - .standardize_conc, 5
 - cleanup_metadata, 19
 - data_model, 21
 - data_model.character, 21
 - data_model.data.table, 22
 - get_assays_per_pipeline_step, 29
 - get_default_nested_identifiers, 29
 - grr_matches, 31
 - identify_keys, 34
 - map_conc_to_standardized_conc, 35
 - order_result_df, 40
 - replace_conc_with_standardized_conc, 44
 - round_concentration, 45
 - .calculate_matrix_metric
(calculate_matrix_metric), 17
 - .map_references, 4
 - .standardize_conc, 5
- add_CellLine_annotation, 6
- add_Drug_annotation, 7
- add_intermediate_data, 8
- average_SE, 9

calculate_Bliss
 (calculate_matrix_metric), 17
calculate_endpt_GR_value
 (calculate_GR_value), 15
calculate_excess, 14
calculate_GR_value, 15
calculate_HSA
 (calculate_matrix_metric), 17
calculate_matrix_metric, 17
calculate_time_dep_GR_value
 (calculate_GR_value), 15
cleanup_metadata, 19
convert_mae_to_raw_data, 20
convert_se_to_raw_data, 20
create_and_normalize_SE (average_SE), 9
create_SE (average_SE), 9

data_model, 21
data_model.character, 21
data_model.data.table, 22
define_matrix_grid_positions, 22
do_skip_step, 23

fit_SE (average_SE), 9
fit_SE.combinations, 23

gDRcore (gDRcore-package), 3
gDRcore-package, 3
generateCodilution, 24
generateCodilutionSmall, 25
generateComboMatrix, 25
generateComboMatrixSmall, 25
generateComboNoNoiseData, 26
generateComboNoNoiseData2, 26
generateComboNoNoiseData3, 26
generateLigandData, 27
generateMediumData, 27
generateNoiseRawData, 27
generateNoNoiseRawData, 28
generateTripleComboMatrix, 28
get_assays_per_pipeline_step, 29
get_default_nested_identifiers, 29
get_mae_from_intermediate_data, 30
get_pipeline_steps, 30
grr_matches, 31

identify_data_type, 32
identify_keys, 34
is_preceding_step, 35

map_conc_to_standardized_conc, 35
map_df, 36
map_ids_to_fits, 38
map_untreated, 39
match, 31
merge, 31
merge_data, 39

normalize_SE (average_SE), 9

order_result_df, 40

prepare_input, 40
prepare_input.data.table, 41
prepare_input.MultiAssayExperiment, 42

read_intermediate_data, 43
remove_drug_batch, 44
replace_conc_with_standardized_conc,
 44
round_concentration, 45
runDrugResponseProcessingPipeline
 (average_SE), 9
runDrugResponseProcessingPipelineFxn
 (average_SE), 9

save_intermediate_data, 46
split_raw_data, 46
SummarizedExperiment, 11, 12, 24

test_synthetic_data, 48