

Package ‘gDRcore’

July 23, 2025

Type Package

Title Processing functions and interface to process and analyze drug dose-response data

Version 1.7.6

Date 2025-07-15

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

Depends R (>= 4.2)

Imports BumpyMatrix, BiocParallel, checkmate, futile.logger, gDRutils (>= 1.7.1), MultiAssayExperiment, purrr, stringr, S4Vectors, SummarizedExperiment, data.table

Suggests BiocStyle, gDRstyle (>= 1.7.1), gDRimport (>= 1.7.1), gDRtestData (>= 1.7.1), IRanges, knitr, pkgbuild, qs, testthat, yaml

VignetteBuilder knitr

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

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

biocViews Software, ShinyApps

ByteCompile TRUE

DeploySubPath gDRcore

Encoding UTF-8

LazyLoad yes

NeedsCompilation yes

RoxygenNote 7.3.2

Roxygen list(markdown = TRUE)

SwitchrLibrary gDRcore

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

git_branch devel

git_last_commit dd1970e

git_last_commit_date 2025-07-15

Repository Bioconductor 3.22

Date/Publication 2025-07-22

Author 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>>),
 Pawel Piatkowski [aut],
 Natalia Potocka [aut],
 Dariusz Scigocki [aut],
 Janina Smola [aut],
 Sergiu Mocanu [aut],
 Marcin Kamianowski [aut],
 Allison Vuong [aut]

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

Contents

gDRcore-package	3
.map_references	4
add_intermediate_data	5
annotate_dt_with_cell_line	5
annotate_dt_with_drug	6
annotate_mae_with_cell_line	7
annotate_mae_with_drug	7
annotate_se_with_cell_line	8
annotate_se_with_drug	9
assert_cell_line_annotation	9
assert_drug_annotation	10
average_SE	10
calculate_excess	15
calculate_GR_value	16
calculate_matrix_metric	18
calculate_score	19
cleanup_metadata	20
convert_mae_to_raw_data	21
convert_se_to_raw_data	21
data_model	22
data_model.character	22
data_model.data.table	23
do_skip_step	23
fit_SE.combinations	24
generateCodilution	25
generateCodilutionSmall	25
generateComboMatrix	25
generateComboMatrixSmall	26
generateComboNoNoiseData	26
generateComboNoNoiseData2	26
generateComboNoNoiseData3	27

generateLigandData	27
generateMediumData	27
generateNoiseRawData	28
generateNoNoiseRawData	28
generateTripleComboMatrix	28
get_assays_per_pipeline_step	29
get_cellline_annotation_from_dt	29
get_cell_line_annotation	30
get_default_nested_identifiers	31
get_drug_annotation	31
get_drug_annotation_from_dt	32
get_mae_from_intermediate_data	33
get_pipeline_steps	33
get_relevant_ids	34
grr_matches	34
identify_data_type	36
identify_keys	37
is_preceding_step	38
map_df	39
map_ids_to_fits	40
map_untreated	41
merge_data	41
order_result_df	42
prepare_input	42
prepare_input.data.table	43
prepare_input.MultiAssayExperiment	44
process_perturbations	45
read_intermediate_data	46
replace_conc_with_standardized_conc	46
save_intermediate_data	47
split_raw_data	48
test_synthetic_data	49
validate_data_models_availability	50

Index	51
--------------	-----------

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

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")`

Author(s)

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

Authors:

- Bartosz Czech <bartosz.czech@contractors.roche.com> ([ORCID](#))
- Marc Hafner ([ORCID](#))
- Pawel Piatkowski
- Natalia Potocka
- Dariusz Scigocki
- Janina Smola
- Sergiu Mocanu
- Marcin Kamianowski
- Allison Vuong

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

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

annotate_dt_with_cell_line
 annotate_dt_with_cell_line

Description

Annotate cell line data with the provided annotation table

Usage

```
annotate_dt_with_cell_line(data, cell_line_annotation, fill = "unknown")
```

Arguments

data	data.table with dose-response data
cell_line_annotation	data.table with cell line annotations
fill	string indicating how unknown cell lines should be filled in the DB

Value

data.table with annotated cell lines

Examples

```
data <- data.table::data.table(
  clid = c("CL1", "CL2", "CL3"),
  Gnumber = c("D1", "D2", "D3")
)
cell_line_annotation <- get_cell_line_annotation(data)
annotated_metadata <- annotate_dt_with_cell_line(data, cell_line_annotation)
```

annotate_dt_with_drug *annotate_dt_with_drug*

Description

Annotate drug data with the provided annotation table

Usage

```
annotate_dt_with_drug(data, drug_annotation, fill = "unknown")
```

Arguments

data	data.table with dose-response data
drug_annotation	data.table with drug annotations
fill	string indicating how unknown drugs should be filled in the DB

Value

data.table with annotated drugs

Examples

```
data <- data.table::data.table(
  clid = c("CL1", "CL2", "CL3"),
  Gnumber = c("D1", "D2", "D3")
)
drug_annotation <- get_drug_annotation(data)
annotated_metadata <- annotate_dt_with_drug(data, drug_annotation)
```

```

annotate_mae_with_cell_line
      annotate_mae_with_cell_line

```

Description

Annotate MultiAssayExperiment object with cell line annotations

Usage

```
annotate_mae_with_cell_line(mae, cell_line_annotation, fill = "unknown")
```

Arguments

mae	MultiAssayExperiment object containing dose-response data
cell_line_annotation	data.table with cell line annotations
fill	string indicating how unknown cell lines should be filled in the DB

Value

MultiAssayExperiment object with annotated cell lines

Examples

```

mae <- MultiAssayExperiment::MultiAssayExperiment(
  experiments = list(exp1 = SummarizedExperiment::SummarizedExperiment(
    rowData = data.table::data.table(clid = c("CL1", "CL2", "CL3"))
  ))
)
cell_line_annotation <- get_cell_line_annotation(data.table::as.data.table(
  SummarizedExperiment::rowData(
    MultiAssayExperiment::experiments(mae)[[1]]
  ))
)
annotated_mae <- annotate_mae_with_cell_line(mae, cell_line_annotation)

```

```

annotate_mae_with_drug
      annotate_mae_with_drug

```

Description

Annotate MultiAssayExperiment object with drug annotations

Usage

```
annotate_mae_with_drug(mae, drug_annotation, fill = "unknown")
```

Arguments

mae MultiAssayExperiment object containing dose-response data
 drug_annotation data.table with drug annotations
 fill string indicating how unknown drugs should be filled in the DB

Value

MultiAssayExperiment object with annotated drugs

Examples

```
mae <- MultiAssayExperiment::MultiAssayExperiment(
  experiments = list(exp1 = SummarizedExperiment::SummarizedExperiment(
    rowData = data.table::data.table(Gnumber = c("D1", "D2", "D3"))
  ))
)
drug_annotation <- get_drug_annotation(data.table::as.data.table(
  SummarizedExperiment::rowData(
    MultiAssayExperiment::experiments(mae)[[1]])))
annotated_mae <- annotate_mae_with_drug(mae, drug_annotation)
```

annotate_se_with_cell_line

annotate_se_with_cell_line

Description

Annotate SummarizedExperiment object with cell line annotations

Usage

```
annotate_se_with_cell_line(se, cell_line_annotation, fill = "unknown")
```

Arguments

se SummarizedExperiment object containing dose-response data
 cell_line_annotation data.table with cell line annotations
 fill string indicating how unknown cell lines should be filled in the DB

Value

SummarizedExperiment object with annotated cell lines

Examples

```
se <- SummarizedExperiment::SummarizedExperiment(
  rowData = data.table::data.table(clid = c("CL1", "CL2", "CL3"))
)
cell_line_annotation <- get_cell_line_annotation(data.table::as.data.table(SummarizedExperiment::rowData(se)))
annotated_se <- annotate_se_with_cell_line(se, cell_line_annotation)
```

annotate_se_with_drug *annotate_se_with_drug*

Description

Annotate SummarizedExperiment object with drug annotations

Usage

```
annotate_se_with_drug(se, drug_annotation, fill = "unknown")
```

Arguments

se	SummarizedExperiment object containing dose-response data
drug_annotation	data.table with drug annotations
fill	string indicating how unknown drugs should be filled in the DB

Value

SummarizedExperiment object with annotated drugs

Examples

```
se <- SummarizedExperiment::SummarizedExperiment(
  rowData = data.table::data.table(Gnumber = c("D1", "D2", "D3"))
)
drug_annotation <- get_drug_annotation(data.table::as.data.table(SummarizedExperiment::rowData(se)))
annotated_se <- annotate_se_with_drug(se, drug_annotation)
```

assert_cell_line_annotation
Assert cell line annotation

Description

Validates that the cell line annotation data.table has the required columns.

Usage

```
assert_cell_line_annotation(cell_line_annotation)
```

Arguments

cell_line_annotation	data.table with cell line annotations
----------------------	---------------------------------------

```
assert_drug_annotation
```

Assert drug annotation

Description

Validates that the drug annotation data.table has the required columns.

Usage

```
assert_drug_annotation(drug_annotation)
```

Arguments

```
drug_annotation
      data.table with drug annotations
```

```
average_SE
```

Run drug response processing pipeline

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,
  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,
  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

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

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 unique 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,
  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")
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",
  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	<i>Calculate a GR value.</i>
--------------------	------------------------------

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")
```

calculate_score	<i>Calculate score for HSA and Bliss</i>
-----------------	--

Description

Calculate score for HSA and Bliss

Usage

```
calculate_score(excess)
```

Arguments

excess	numeric vector with excess
--------	----------------------------

Value

numeric vector with calculated score

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"  
x <- calculate_excess(  
  metric,  
  measured,  
  series_identifiers,  
  metric_col,  
  measured_col  
)  
calculate_score(x$x)
```

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

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

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 *fit_SE for combination screens*

Description

Perform fittings for combination screens.

Usage

```
fit_SE.combinations(
  se,
  data_type = gDRutils::get_supported_experiments("combo"),
  series_identifiers = NULL,
  normalization_types = c("GR", "RV"),
  averaged_assay = "Averaged",
  metrics_assay = "Metrics",
  score_FUN = calculate_score
)
```

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.
score_FUN	function used to calculate score for HSA and Bliss

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_supported_experiments("combo")]]
SummarizedExperiment::assays(se1) <-
  SummarizedExperiment::assays(se1)["Averaged"]
fit_SE.combinations(se1[1, 1])
```

generateCodilution	<i>generateCodilution</i>
--------------------	---------------------------

Description

generateCodilution

Usage

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

Value

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

generateCodilutionSmall	<i>generateCodilutionSmall</i>
-------------------------	--------------------------------

Description

generateCodilutionSmall

Usage

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

Value

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

generateComboMatrix	<i>generateComboMatrix</i>
---------------------	----------------------------

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	<i>generateNoiseRawData</i>
----------------------	-----------------------------

Description

generateNoiseRawData

Usage

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

Value

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

generateNoNoiseRawData	<i>generateNoNoiseRawData</i>
------------------------	-------------------------------

Description

generateNoNoiseRawData

Usage

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

Value

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

generateTripleComboMatrix	<i>generateTripleComboMatrix</i>
---------------------------	----------------------------------

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_cellline_annotation_from_dt`*Retrieve the cell line annotation from the annotated dt input*

Description

Retrieve the cell line annotation from the annotated dt input

Usage

```
get_cellline_annotation_from_dt(dt)
```

Arguments

dt	annotated data.table
----	----------------------

Value

data.table with cell line annotation

Examples

```
dt <- data.table::data.table(Gnumber = "A",
  clid = "CL123",
  CellLineName = "cl name",
  Tissue = "Bone",
  parental_identifier = "some cl",
  subtype = "cortical",
  ReferenceDivisionTime = 5)
get_cellline_annotation_from_dt(dt)
```

```
get_cell_line_annotation
      get_cell_line_annotation
```

Description

Get cell line annotation data table

Usage

```
get_cell_line_annotation(
  data,
  fname = "cell_lines.csv",
  fill = "unknown",
  annotation_package = if ("gDRinternal" %in% .packages(all.available = TRUE)) {
    "gDRinternal"
  } else {
    "gDRtestData"
  }
)
```

Arguments

data	data.table with cell line identifiers to be matched
fname	string with file name containing the annotation
fill	string indicating how unknown cell lines should be filled in the DB
annotation_package	string indicating name of the package containing cell line annotation

Value

data.table with cell line annotations

Examples

```
data <- data.table::data.table(clid = c("CL1", "CL2", "CL3"))
cell_line_annotation <- get_cell_line_annotation(data)
```

```
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_drug_annotation      get_drug_annotation
```

Description

Get drug annotation data table

Usage

```
get_drug_annotation(
  data,
  fname = "drugs.csv",
  fill = "unknown",
  annotation_package = if ("gDRinternal" %in% .packages(all.available = TRUE)) {
    "gDRinternal"
  } else {
    "gDRtestData"
  }
)
```

Arguments

data	data.table with drug identifiers to be matched
fname	string with file name containing the annotation
fill	string indicating how unknown drugs should be filled in the DB
annotation_package	string indicating name of the package containing drug annotation

Value

data.table with drug annotations

Examples

```
data <- data.table::data.table(Gnumber = c("drug1", "drug2", "drug3"))
drug_annotation <- get_drug_annotation(data)
```

```
get_drug_annotation_from_dt
```

Retrieve the drug annotation from the annotated dt input

Description

Retrieve the drug annotation from the annotated dt input

Usage

```
get_drug_annotation_from_dt(dt)
```

Arguments

dt	annotated data.table
----	----------------------

Value

data.table with drug annotation

Examples

```
dt <- data.table::data.table(Gnumber = "A",
DrugName = "drugA",
drug_moa = "drug_moa_A")
get_drug_annotation_from_dt(dt)
```

get_mae_from_intermediate_data	
	<i>get mae dataset from intermediate data</i>

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	<i>get pipeline steps</i>
--------------------	---------------------------

Description

get pipeline steps

Usage

```
get_pipeline_steps()
```

Value

vector with steps

get_relevant_ids	<i>Function to get relevant identifiers from the environment</i>
------------------	--

Description

Function to get relevant identifiers from the environment

Usage

```
get_relevant_ids(identifiers, dt)
```

Arguments

identifiers	A character vector of identifier names to fetch from the environment
dt	A data.table containing the columns to be checked against the identifiers

Value

A character vector of relevant identifiers that are present in the data.table

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

<code>list</code>	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.
<code>indexes</code>	logical. Whether to return the indices of the matches or the actual values.
<code>nomatch</code>	the value to be returned in the case when no match is found. If not provided and <code>indexes=TRUE</code> , 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 <code>length+1</code> . If <code>indexes=FALSE</code> , 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	<i>Identify type of data</i>
--------------------	------------------------------

Description

Identify type of data

Usage

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

Arguments

dt	data.table of raw drug response data containing both treated and untreated values
codilution_conc	integer of maximum number of concentration ratio of co-treatment to classify as codilution data type; defaults to 2
matrix_conc	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_dt <- 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_dt <- S4Vectors::DataFrame(
  ReadoutValue = rep(seq(1, 4, 1), 2),
  Concentration = conc,
  masked = rep(FALSE, 8),
  DrugName = c("DRUG_10", "DRUG_8"),
  CellLineName = "CELL1"
)

```

```

)
input_dt <- data.table::as.data.table(rbind(ctrl_dt, trt_dt))
input_dt$Duration <- 72
input_dt$CorrectedReadout2 <- input_dt$ReadoutValue
identify_data_type(input_dt)

```

identify_keys

identify_keys

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

<code>df_</code>	a data.table to identify keys for.
<code>nested_keys</code>	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.
<code>override_untrt_controls</code>	named list containing defining factors in the treatments. Defaults to NULL.
<code>identifiers</code>	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_identifier = "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_df	<i>Map treated conditions to their respective references.</i>
--------	---

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

Get predicted values for a given fit and input.

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 treaatments 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-response 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-response 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

process_perturbations *Cleanup additional perturbations in the data.table*

Description

This function processes drug and concentration columns in a data.table. It checks if there is only one unique drug (excluding a specified untreated tag) and if there are exactly two doses (one of which is 0). If these conditions are met, it creates a new column named after the drug and fills it with the doses, then removes the original drug and concentration columns.

Usage

```
process_perturbations(
  dt,
  drugs_cotrt_ids,
  conc_cotrt_ids,
  untreated_tag = "vehicle"
)
```

Arguments

dt A data.table containing the data.

drugs_cotrt_ids A vector of column names related to drugs.

conc_cotrt_ids A vector of column names related to concentrations.

untreated_tag A string representing the untreated tag (default is "vehicle").

Value

A modified data.table with new columns for the drugs and removed original drug and concentration columns.

Examples

```
dt <- data.table::data.table(
  drug1 = c("vehicle", "drugA", "drugA"),
  conc1 = c(0, 10, 0),
  drug2 = c("vehicle", "drugB", "drugB"),
  conc2 = c(0, 20, 0)
)
drugs_cotrt_ids <- c("drug1", "drug2")
conc_cotrt_ids <- c("conc1", "conc2")
dt <- process_perturbations(dt, drugs_cotrt_ids, conc_cotrt_ids)
print(dt)
```

```
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

```
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"
)
```

`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	<i>Split raw data into list based on the data types</i>
----------------	---

Description

Split raw data into list based on the data types

Usage

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

Arguments

dt 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 `dt` with info about data type. Defaults to "type".

Value

list with split data based on its data type

Author(s)

Bartosz Czech bartosz.czech@contractors.rocche.com

Examples

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

dt_2 <-
  drugs[c(21, 26), as.list(cell_lines[which(cell_lines$clid %in% dt_layout$clid)]), names(drugs)]
dt_2 <- gDRtestData::add_data_replicates(dt_2)
dt_2 <- gDRtestData::add_concentration(
  dt_2,
  concentrations = 10 ^ (seq(-3, .5, .5))
)
colnames(dt_2)[colnames(dt_2) %in% c(colnames(drugs), "Concentration")] <-
  paste0(
    colnames(dt_2)[colnames(dt_2) %in% c(colnames(drugs), "Concentration")],
    "_2"
  )
dt_layout_2 <- dt_layout[dt_2, on = intersect(names(dt_layout), names(dt_2)),
  allow.cartesian = TRUE]
```

```

dt_merged_data <- gDRtestData::generate_response_data(dt_layout_2, 0)
dt <- identify_data_type(dt_merged_data)
split_raw_data(dt)

conc <- rep(seq(0, 0.3, 0.1), 2)
ctrl_dt <- 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_dt <- S4Vectors::DataFrame(
  ReadoutValue = rep(seq(1, 4, 1), 2),
  Concentration = conc,
  masked = rep(FALSE, 8),
  DrugName = c("DRUG_10", "DRUG_8"),
  CellLineName = "CELL1"
)
input_dt <- data.table::as.data.table(rbind(ctrl_dt, trt_dt))
input_dt$Duration <- 72
input_dt$CorrectedReadout2 <- input_dt$ReadoutValue
split_dt <- identify_data_type(input_dt)
split_raw_data(split_dt)

```

test_synthetic_data	<i>Testing synthetic data form gDRtestData package</i>
---------------------	--

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")
```

`validate_data_models_availability`*Validate availability of data models*

Description

Validate availability of data models

Usage`validate_data_models_availability(d_types, s_d_models)`**Arguments**

<code>d_types</code>	character vector with experiment names in MultiAssayExperiment object
<code>s_d_models</code>	character vector with names of supported experiment

Index

- * **annotation**
 - annotate_dt_with_cell_line, 5
 - annotate_dt_with_drug, 6
 - annotate_mae_with_cell_line, 7
 - annotate_mae_with_drug, 7
 - annotate_se_with_cell_line, 8
 - annotate_se_with_drug, 9
 - get_cell_line_annotation, 30
 - get_cellline_annotation_from_dt, 29
 - get_drug_annotation, 31
 - get_drug_annotation_from_dt, 32
- * **calculate_GR**
 - calculate_GR_value, 16
- * **combinations**
 - calculate_excess, 15
 - calculate_matrix_metric, 18
 - calculate_score, 19
- * **convert_to_raw_data**
 - convert_mae_to_raw_data, 21
 - convert_se_to_raw_data, 21
- * **data_type**
 - identify_data_type, 36
 - process_perturbations, 45
 - split_raw_data, 48
- * **internal**
 - add_intermediate_data, 5
 - assert_cell_line_annotation, 9
 - assert_drug_annotation, 10
 - do_skip_step, 23
 - gDRcore-package, 3
 - generateCodilution, 25
 - generateCodilutionSmall, 25
 - generateComboMatrix, 25
 - generateComboMatrixSmall, 26
 - generateComboNoNoiseData, 26
 - generateComboNoNoiseData2, 26
 - generateComboNoNoiseData3, 27
 - generateLigandData, 27
 - generateMediumData, 27
 - generateNoiseRawData, 28
 - generateNoNoiseRawData, 28
 - generateTripleComboMatrix, 28
 - get_mae_from_intermediate_data, 33
 - get_pipeline_steps, 33
 - get_relevant_ids, 34
 - is_preceding_step, 38
 - read_intermediate_data, 46
 - save_intermediate_data, 47
 - validate_data_models_availability, 50
- * **map_df**
 - .map_references, 4
 - map_df, 39
 - map_ids_to_fits, 40
 - map_untreated, 41
- * **merge_data**
 - merge_data, 41
- * **prepare_input**
 - prepare_input, 42
 - prepare_input.data.table, 43
 - prepare_input.MultiAssayExperiment, 44
- * **runDrugResponseProcessingPipeline**
 - average_SE, 10
 - fit_SE.combinations, 24
- * **test_utils**
 - test_synthetic_data, 49
- * **utils**
 - cleanup_metadata, 20
 - data_model, 22
 - data_model.character, 22
 - data_model.data.table, 23
 - get_assays_per_pipeline_step, 29
 - get_default_nested_identifiers, 31
 - grr_matches, 34
 - identify_keys, 37
 - order_result_df, 42
 - replace_conc_with_standardized_conc, 46
 - .calculate_matrix_metric (calculate_matrix_metric), 18
 - .map_references, 4
 - add_intermediate_data, 5
 - annotate_dt_with_cell_line, 5
 - annotate_dt_with_drug, 6

annotate_mae_with_cell_line, 7
 annotate_mae_with_drug, 7
 annotate_se_with_cell_line, 8
 annotate_se_with_drug, 9
 assert_cell_line_annotation, 9
 assert_drug_annotation, 10
 average_SE, 10

 calculate_Bliss
 (calculate_matrix_metric), 18
 calculate_endpt_GR_value
 (calculate_GR_value), 16
 calculate_excess, 15
 calculate_GR_value, 16
 calculate_HSA
 (calculate_matrix_metric), 18
 calculate_matrix_metric, 18
 calculate_score, 19
 calculate_time_dep_GR_value
 (calculate_GR_value), 16
 cleanup_metadata, 20
 convert_mae_to_raw_data, 21
 convert_se_to_raw_data, 21
 create_and_normalize_SE (average_SE), 10
 create_SE (average_SE), 10

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

 fit_SE (average_SE), 10
 fit_SE.combinations, 24

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

 get_drug_annotation_from_dt, 32
 get_mae_from_intermediate_data, 33
 get_pipeline_steps, 33
 get_relevant_ids, 34
 grr_matches, 34

 identify_data_type, 36
 identify_keys, 37
 is_preceding_step, 38

 map_df, 39
 map_ids_to_fits, 40
 map_untreated, 41
 match, 34
 merge, 35
 merge_data, 41

 normalize_SE (average_SE), 10

 order_result_df, 42

 prepare_input, 42
 prepare_input.data.table, 43
 prepare_input.MultiAssayExperiment, 44
 process_perturbations, 45

 read_intermediate_data, 46
 replace_conc_with_standardized_conc,
 46
 runDrugResponseProcessingPipeline
 (average_SE), 10
 runDrugResponseProcessingPipelineFxns
 (average_SE), 10

 save_intermediate_data, 47
 split_raw_data, 48
 SummarizedExperiment, 12, 13, 24

 test_synthetic_data, 49

 validate_data_models_availability, 50