

# Package ‘gDRcore’

February 17, 2025

**Type** Package

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

**Version** 1.4.4

**Date** 2025-01-13

**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 (>= 1.4.6), MultiAssayExperiment, purrr, stringr, S4Vectors, SummarizedExperiment, data.table

**Suggests** BiocStyle, gDRstyle (>= 1.1.5), gDRimport (>= 1.1.9), gDRtestData (>= 1.1.10), 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** RELEASE\_3\_20

**git\_last\_commit** cf001e6

**git\_last\_commit\_date** 2025-02-11

**Repository** Bioconductor 3.20

**Date/Publication** 2025-02-17

**Author** Bartosz Czech [aut] (<<https://orcid.org/0000-0002-9908-3007>>),  
 Arkadiusz Gladki [cre, aut] (<<https://orcid.org/0000-0002-7059-6378>>),  
 Marc Hafner [aut] (<<https://orcid.org/0000-0003-1337-7598>>),  
 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](mailto:gladki.arkadiusz@gmail.com)>

## Contents

gDRcore-package . . . . .	3
.map_references . . . . .	4
.standardize_conc . . . . .	5
add_intermediate_data . . . . .	5
annotate_dt_with_cell_line . . . . .	6
annotate_dt_with_drug . . . . .	6
average_SE . . . . .	7
calculate_excess . . . . .	12
calculate_GR_value . . . . .	13
calculate_matrix_metric . . . . .	15
calculate_score . . . . .	16
cleanup_metadata . . . . .	17
convert_mae_to_raw_data . . . . .	18
convert_se_to_raw_data . . . . .	18
data_model . . . . .	19
data_model.character . . . . .	19
data_model.data.table . . . . .	20
do_skip_step . . . . .	20
fit_SE.combinations . . . . .	21
generateCodilution . . . . .	22
generateCodilutionSmall . . . . .	22
generateComboMatrix . . . . .	22
generateComboMatrixSmall . . . . .	23
generateComboNoNoiseData . . . . .	23
generateComboNoNoiseData2 . . . . .	23
generateComboNoNoiseData3 . . . . .	24
generateLigandData . . . . .	24
generateMediumData . . . . .	24
generateNoiseRawData . . . . .	25
generateNoNoiseRawData . . . . .	25
generateTripleComboMatrix . . . . .	25
get_assays_per_pipeline_step . . . . .	26

get_cellline_annotation_from_dt . . . . .	26
get_cell_line_annotation . . . . .	27
get_default_nested_identifiers . . . . .	28
get_drug_annotation . . . . .	28
get_drug_annotation_from_dt . . . . .	29
get_mae_from_intermediate_data . . . . .	30
get_pipeline_steps . . . . .	30
get_relevant_ids . . . . .	31
grr_matches . . . . .	31
identify_data_type . . . . .	33
identify_keys . . . . .	34
is_preceding_step . . . . .	35
map_conc_to_standardized_conc . . . . .	36
map_df . . . . .	37
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
process_perturbations . . . . .	43
read_intermediate_data . . . . .	44
replace_conc_with_standardized_conc . . . . .	44
save_intermediate_data . . . . .	45
split_raw_data . . . . .	46
test_synthetic_data . . . . .	47
validate_data_models_availability . . . . .	48

**Index****49**


---

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

---

.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\_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)
```

---

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,
  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	<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

`rel_viability` numeric vector representing the Relative Viability.

`corrected_readout` numeric vector containing the corrected readout.

`day0_readout` numeric vector containing the day 0 readout.

`untrt_readout` numeric vector containing the untreated readout.

`ndigit_rounding` integer specifying the number of digits to use for calculation rounding.

`duration` numeric value specifying the length of time the cells were treated (in hours).

`ref_div_time` numeric value specifying the reference division time for the cell line in the experiment.

`cap` 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.n 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

*Calculate score for HSA and Bliss*

---

### 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 *Detect model of data*

---

**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 *Detect model of data from experiment name*

---

**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 <a href="#">SummarizedExperiment</a> . 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    *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_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  
*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

---

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 <code>y</code> . If FALSE, result is returned as a <code>data.table</code> 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      *Identify type of data*

---

### 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](mailto: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

`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_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_conc_to_standardized_conc
```

*Create a mapping of concentrations to standardized concentrations.*

---

### 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	<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_identifiser = "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 treatments 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.roche.com](mailto:bartosz.czech@contractors.roche.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     *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")
```

---

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



# Index

- \* **annotation**
  - annotate\_dt\_with\_cell\_line, 6
  - annotate\_dt\_with\_drug, 6
  - get\_cell\_line\_annotation, 27
  - get\_cellline\_annotation\_from\_dt, 26
  - get\_drug\_annotation, 28
  - get\_drug\_annotation\_from\_dt, 29
- \* **calculate\_GR**
  - calculate\_GR\_value, 13
- \* **combinations**
  - calculate\_excess, 12
  - calculate\_matrix\_metric, 15
  - calculate\_score, 16
- \* **convert\_to\_raw\_data**
  - convert\_mae\_to\_raw\_data, 18
  - convert\_se\_to\_raw\_data, 18
- \* **data\_type**
  - identify\_data\_type, 33
  - process\_perturbations, 43
  - split\_raw\_data, 46
- \* **internal**
  - add\_intermediate\_data, 5
  - do\_skip\_step, 20
  - gDRcore-package, 3
  - generateCodilution, 22
  - generateCodilutionSmall, 22
  - generateComboMatrix, 22
  - generateComboMatrixSmall, 23
  - generateComboNoNoiseData, 23
  - generateComboNoNoiseData2, 23
  - generateComboNoNoiseData3, 24
  - generateLigandData, 24
  - generateMediumData, 24
  - generateNoiseRawData, 25
  - generateNoNoiseRawData, 25
  - generateTripleComboMatrix, 25
  - get\_mae\_from\_intermediate\_data, 30
  - get\_pipeline\_steps, 30
  - get\_relevant\_ids, 31
  - is\_preceding\_step, 35
  - read\_intermediate\_data, 44
  - save\_intermediate\_data, 45
  - validate\_data\_models\_availability, 48
- \* **map\_df**
  - .map\_references, 4
  - map\_df, 37
  - 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, 7
  - fit\_SE.combinations, 21
- \* **test\_utils**
  - test\_synthetic\_data, 47
- \* **utils**
  - .standardize\_conc, 5
  - cleanup\_metadata, 17
  - data\_model, 19
  - data\_model.character, 19
  - data\_model.data.table, 20
  - get\_assays\_per\_pipeline\_step, 26
  - get\_default\_nested\_identifiers, 28
  - grr\_matches, 31
  - identify\_keys, 34
  - map\_conc\_to\_standardized\_conc, 36
  - order\_result\_df, 40
  - replace\_conc\_with\_standardized\_conc, 44
  - .calculate\_matrix\_metric (calculate\_matrix\_metric), 15
  - .map\_references, 4
  - .standardize\_conc, 5
  - add\_intermediate\_data, 5
  - annotate\_dt\_with\_cell\_line, 6
  - annotate\_dt\_with\_drug, 6
  - average\_SE, 7
  - calculate\_Bliss

(calculate\_matrix\_metric), 15  
calculate\_endpt\_GR\_value  
    (calculate\_GR\_value), 13  
calculate\_excess, 12  
calculate\_GR\_value, 13  
calculate\_HSA  
    (calculate\_matrix\_metric), 15  
calculate\_matrix\_metric, 15  
calculate\_score, 16  
calculate\_time\_dep\_GR\_value  
    (calculate\_GR\_value), 13  
cleanup\_metadata, 17  
convert\_mae\_to\_raw\_data, 18  
convert\_se\_to\_raw\_data, 18  
create\_and\_normalize\_SE (average\_SE), 7  
create\_SE (average\_SE), 7  
  
data\_model, 19  
data\_model.character, 19  
data\_model.data.table, 20  
do\_skip\_step, 20  
  
fit\_SE (average\_SE), 7  
fit\_SE.combinations, 21  
  
gDRcore (gDRcore-package), 3  
gDRcore-package, 3  
generateCodilution, 22  
generateCodilutionSmall, 22  
generateComboMatrix, 22  
generateComboMatrixSmall, 23  
generateComboNoNoiseData, 23  
generateComboNoNoiseData2, 23  
generateComboNoNoiseData3, 24  
generateLigandData, 24  
generateMediumData, 24  
generateNoiseRawData, 25  
generateNoNoiseRawData, 25  
generateTripleComboMatrix, 25  
get\_assays\_per\_pipeline\_step, 26  
get\_cell\_line\_annotation, 27  
get\_cellline\_annotation\_from\_dt, 26  
get\_default\_nested\_identifiers, 28  
get\_drug\_annotation, 28  
get\_drug\_annotation\_from\_dt, 29  
get\_mae\_from\_intermediate\_data, 30  
get\_pipeline\_steps, 30  
get\_relevant\_ids, 31  
grr\_matches, 31  
  
identify\_data\_type, 33  
identify\_keys, 34  
is\_preceding\_step, 35  
  
map\_conc\_to\_standardized\_conc, 36  
map\_df, 37  
map\_ids\_to\_fits, 38  
map\_untreated, 39  
match, 31  
merge, 32  
merge\_data, 39  
  
normalize\_SE (average\_SE), 7  
  
order\_result\_df, 40  
  
prepare\_input, 40  
prepare\_input.data.table, 41  
prepare\_input.MultiAssayExperiment, 42  
process\_perturbations, 43  
  
read\_intermediate\_data, 44  
replace\_conc\_with\_standardized\_conc,  
    44  
runDrugResponseProcessingPipeline  
    (average\_SE), 7  
runDrugResponseProcessingPipelineFxns  
    (average\_SE), 7  
  
save\_intermediate\_data, 45  
split\_raw\_data, 46  
SummarizedExperiment, 9, 10, 21  
  
test\_synthetic\_data, 47  
  
validate\_data\_models\_availability, 48