

# Package: gDRcore (via r-universe)

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**Type** Package

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

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

**License** Artistic-2.0

**Depends** R (>= 4.2)

**Imports** BumpyMatrix, BiocParallel, checkmate, futile.logger, gDRutils (>= 1.1.14), MultiAssayExperiment, purrr, stringr, S4Vectors, SummarizedExperiment, data.table

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**VignetteBuilder** knitr

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

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

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## Contents

.map_references . . . . .	3
.standardize_conc . . . . .	3
add_CellLine_annotation . . . . .	4
add_Drug_annotation . . . . .	5
average_SE . . . . .	6
calculate_excess . . . . .	12
calculate_GR_value . . . . .	13
calculate_matrix_metric . . . . .	15
cleanup_metadata . . . . .	16
convert_mae_to_raw_data . . . . .	17
convert_se_to_raw_data . . . . .	18
data_model . . . . .	18
data_model.character . . . . .	19
data_model.data.table . . . . .	19
fit_SE.combinations . . . . .	20
get_assays_per_pipeline_step . . . . .	21
get_cellline_annotation_from_dt . . . . .	21
get_default_nested_identifiers . . . . .	22
get_drug_annotation_from_dt . . . . .	23
grr_matches . . . . .	23
identify_data_type . . . . .	25
identify_keys . . . . .	26
map_conc_to_standardized_conc . . . . .	27
map_df . . . . .	28
map_ids_to_fits . . . . .	30
map_untreated . . . . .	31
merge_data . . . . .	31
order_result_df . . . . .	32
prepare_input . . . . .	32
prepare_input.data.table . . . . .	33
prepare_input.MultiAssayExperiment . . . . .	34
remove_drug_batch . . . . .	35
replace_conc_with_standardized_conc . . . . .	36
split_raw_data . . . . .	37
test_synthetic_data . . . . .	38

## Index

40

---

.map\_references      *Map references*

---

### Description

Map references

### Usage

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

### Arguments

mat\_elem      input data frame  
rowData\_colnames      character vector of variables for the mapping of reference treatments

### Details

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

### Value

list

---

.standardize\_conc      *Standardize concentration values.*

---

### Description

Standardize concentration values.

### Usage

```
.standardize_conc(conc)
```

### Arguments

conc      numeric vector of the concentrations

### Details

If no conc are passed, NULL is returned.

**Value**

vector of standardized concentrations

**Examples**

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

---

```
add_CellLine_annotation
      add_CellLine_annotation
```

---

**Description**

add cellline annotation to a data.table with metadata

**Usage**

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

**Arguments**

dt_metadata	data.table with metadata
DB_cellid_header	string with colnames with cell line identifier in the annotation file
DB_cell_annotate	character vector with mandatory colnames used in the annotation file
fname	string with file name with annotation
fill	string indicating how unknown cell lines should be filled in the DB
annotation_package	string indication name of the package containing cellline annotation

external\_source

string with path to external file with annotation data; by default it checks 'GDR\_CELLLINE\_ANNOTATION' env var. This file should contain columns such as gnumber, drug\_name and drug\_moa

## Details

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

## Value

data.table with metadata with annotated cell lines

## Examples

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

---

add\_Drug\_annotation    *add\_Drug\_annotation*

---

## Description

add drug annotation to a data.table with metadata

## Usage

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

**Arguments**

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

**Details**

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

**Value**

data.table with metadata with annotated drugs

**Examples**

```

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

```

---

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 <a href="#">SummarizedExperiment</a> . 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 <a href="#">SummarizedExperiment</a> 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 uniquenested\_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	<i>Calculate the difference between values in two data.tables</i>
------------------	---

---

### 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.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")
```

---

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

---

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"
)
```

## 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.

## 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])
```

---

*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_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_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)
```

---

`grr_matches`*Value Matching*

---

**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

<code>x</code>	vector. The values to be matched. Long vectors are not currently supported.
<code>y</code>	vector. The values to be matched. Long vectors are not currently supported.
<code>all.x</code>	logical; if TRUE, then each value in <code>x</code> will be included even if it has no matching values in <code>y</code>
<code>all.y</code>	logical; if TRUE, then each value in <code>y</code> will be included even if it has no matching values in <code>x</code>
<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 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      *Identify type of data*

---

## Description

Identify type of data

## Usage

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

## Arguments

df	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_df <- S4Vectors::DataFrame(
  ReadoutValue = c(2, 2, 1, 1, 2, 1),
  Concentration = rep(0, 6),
  masked = FALSE,
  DrugName = rep(c("DRUG_10", "vehicle", "DRUG_8"), 2),
  CellLineName = "CELL1"
)

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

```

---

identify\_keys

*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)
```

---

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

*Map treated conditions to their respective references.*

---

**Description**

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

**Usage**

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

**Arguments**

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

**Details**

If override\_untrt\_controls is specified, TODO: FILL ME!

**Value**

named list mapping treated metadata to untreated metadata.

**See Also**

identify\_keys

**Examples**

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

---

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

---

## Description

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

## Usage

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

## Arguments

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

## Value

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

## Examples

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

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

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

---

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

---

**Description**

Identify untreated rows based on Drug treatment alone

**Usage**

```
map_untreated(mat_elem)
```

**Arguments**

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

**Details**

Using the given rownames, map the untreated conditions

**Value**

list

---

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

---

**Description**

Merge all the input data into a single data.table

**Usage**

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

**Arguments**

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

**Value**

a data.table with merged data and metadata.

**Examples**

```

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

```

---

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

---

**Description**

Order a data.table with results

**Usage**

```
order_result_df(df_)
```

**Arguments**

df\_ a data.table with results

**Value**

a ordered data.table with results

---

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

---

**Description**

Current steps

- refining nested confounders
- refining nested identifiers
- splitting df\_ into (per experiment) df\_list

**Usage**

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



**Arguments**

x                    data.table with raw data or MAE object with dose-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

---

remove_drug_batch	<i>Remove batch from Gnumber</i>
-------------------	----------------------------------

---

**Description**

Remove batch from Gnumber

**Usage**

```
remove_drug_batch(drug)
```

**Arguments**

drug	drug name
------	-----------

**Value**

Gnumber without a batch

**Examples**

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

---

```
replace_conc_with_standardized_conc
```

*Standardize concentrations.*

---

### Description

Utilize a map to standardize concentrations.

### Usage

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

### Arguments

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

### Value

numeric vector of standardized concentrations.

### See Also

`map_conc_to_standardized_conc`

### Examples

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

```

    standardized_conc_col = "std"
  )

```

---

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

## Arguments

df	data.table of raw drug response data containing both treated and untreated values with column specified in type_col argument.
type_col	string with column names in df with info about data type. Defaults to "type".

## Value

list with split data based on its data type

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

df_2 <-
  drugs[c(21, 26), as.list(cell_lines[which(cell_lines$clid %in% df_layout$clid)]), names(drugs)]
df_2 <- gDRtestData::add_data_replicates(df_2)
df_2 <- gDRtestData::add_concentration(
  df_2,
  concentrations = 10 ^ (seq(-3, .5, .5))
)
colnames(df_2)[colnames(df_2) %in% c(colnames(drugs), "Concentration")] <-
  paste0(
    colnames(df_2)[colnames(df_2) %in% c(colnames(drugs), "Concentration")],

```

```

    "_2"
  )
df_layout_2 <- df_layout[df_2, on = intersect(names(df_layout), names(df_2)),
  allow.cartesian = TRUE]
df_merged_data <- gDRtestData::generate_response_data(df_layout_2, 0)
df <- identify_data_type(df_merged_data)
split_raw_data(df)

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

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

```

---

test\_synthetic\_data    *Testing synthetic data form gDRtestData package*

---

## Description

Testing synthetic data form gDRtestData package

## Usage

```

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

```

**Arguments**

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

**Value**

NULL

**Examples**

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

# Index

- \* **annotation**
  - add\_CellLine\_annotation, 4
  - add\_Drug\_annotation, 5
  - get\_cellline\_annotation\_from\_dt, 21
  - get\_drug\_annotation\_from\_dt, 23
  - remove\_drug\_batch, 35
- \* **calculate\_GR**
  - calculate\_GR\_value, 13
- \* **combinations**
  - calculate\_excess, 12
  - calculate\_matrix\_metric, 15
- \* **convert\_to\_raw\_data**
  - convert\_mae\_to\_raw\_data, 17
  - convert\_se\_to\_raw\_data, 18
- \* **data\_type**
  - identify\_data\_type, 25
  - split\_raw\_data, 37
- \* **map\_df**
  - .map\_references, 3
  - map\_df, 28
  - map\_ids\_to\_fits, 30
  - map\_untreated, 31
- \* **merge\_data**
  - merge\_data, 31
- \* **prepare\_input**
  - prepare\_input, 32
  - prepare\_input.data.table, 33
  - prepare\_input.MultiAssayExperiment, 34
- \* **runDrugResponseProcessingPipeline**
  - average\_SE, 6
  - fit\_SE.combinations, 20
- \* **test\_utils**
  - test\_synthetic\_data, 38
- \* **utils**
  - .standardize\_conc, 3
  - cleanup\_metadata, 16
  - data\_model, 18
  - data\_model.character, 19
  - data\_model.data.table, 19
  - data\_model.character, 19
  - data\_model.data.table, 19
  - get\_assays\_per\_pipeline\_step, 21
  - get\_default\_nested\_identifiers, 22
  - grr\_matches, 23
  - identify\_keys, 26
  - map\_conc\_to\_standardized\_conc, 27
  - order\_result\_df, 32
  - replace\_conc\_with\_standardized\_conc, 36
  - .calculate\_matrix\_metric (calculate\_matrix\_metric), 15
  - .map\_references, 3
  - .standardize\_conc, 3
  - add\_CellLine\_annotation, 4
  - add\_Drug\_annotation, 5
  - average\_SE, 6
  - 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\_time\_dep\_GR\_value (calculate\_GR\_value), 13
  - cleanup\_metadata, 16
  - convert\_mae\_to\_raw\_data, 17
  - convert\_se\_to\_raw\_data, 18
  - create\_and\_normalize\_SE (average\_SE), 6
  - create\_SE (average\_SE), 6
  - data\_model, 18
  - data\_model.character, 19
  - data\_model.data.table, 19
  - fit\_SE (average\_SE), 6



fit\_SE.combinations, 20

get\_assays\_per\_pipeline\_step, 21  
get\_cellline\_annotation\_from\_dt, 21  
get\_default\_nested\_identifiers, 22  
get\_drug\_annotation\_from\_dt, 23  
grr\_matches, 23

identify\_data\_type, 25  
identify\_keys, 26

map\_conc\_to\_standardized\_conc, 27  
map\_df, 28  
map\_ids\_to\_fits, 30  
map\_untreated, 31  
match, 23  
merge, 24  
merge\_data, 31

normalize\_SE (average\_SE), 6

order\_result\_df, 32

prepare\_input, 32  
prepare\_input.data.table, 33  
prepare\_input.MultiAssayExperiment, 34

remove\_drug\_batch, 35  
replace\_conc\_with\_standardized\_conc,  
36

runDrugResponseProcessingPipeline  
(average\_SE), 6  
runDrugResponseProcessingPipelineFxn  
(average\_SE), 6

split\_raw\_data, 37  
SummarizedExperiment, 8–10, 20

test\_synthetic\_data, 38