

# Package: gDRutils (via r-universe)

July 5, 2024

**Type** Package

**Title** A package with helper functions for processing drug response data

**Version** 1.3.3

**Date** 2024-07-03

**Description** This package contains utility functions used throughout the gDR platform to fit data, manipulate data, and convert and validate data structures. This package also has the necessary default constants for gDR platform. Many of the functions are utilized by the gDRcore package.

**License** Artistic-2.0

**LazyLoad** yes

**Depends** R (>= 4.2)

**Imports** BiocParallel, BumpyMatrix, checkmate, data.table, drc, jsonlite, jsonvalidate, methods, MultiAssayExperiment, S4Vectors, stats, stringr, SummarizedExperiment

**Suggests** BiocManager, BiocStyle, futile.logger, gDRstyle (>= 1.1.5), gDRtestData (>= 1.1.10), IRanges, knitr, lintr, purrr, qs, rcmdcheck, rmarkdown, scales, testthat, tools, yaml

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

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

**biocViews** Software, Infrastructure

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---

`.set_invalid_fit_params`

*Set fit parameters for an invalid fit.*

---

## Description

Set fit parameters for an invalid fit.

## Usage

```
.set_invalid_fit_params(out, norm_values)
```

## Arguments

`out`                Named list of fit parameters.

`norm_values`      Numeric vector used to estimate an `xc50` value.

## Value

Modified named list of fit parameters.

## Examples

```
.set_invalid_fit_params(list(), norm_values = rep(0.3, 6))
```

---

addClass	<i>add arbitrary S3 class to an object</i>
----------	--

---

**Description**

Modify and object's class attribute.

**Usage**

```
addClass(x, newClass)
```

**Arguments**

x	an object
newClass	character string; class to be added

**Details**

This is a simple convenience function that an item to the class attribute of an object so that it can be dispatched to a proper S3 method. This is purely for code clarity, so that individual methods do not clutter the definitions of higher order functions.

**Value**

The same object with an added S3 class.

**Examples**

```
addClass(data.table::data.table(), "someClass")
```

---

aggregate_assay	<i>Aggregate a BumpyMatrix assay by a given aggregation function.</i>
-----------------	---

---

**Description**

Aggregation can only be performed on nested variables.

**Usage**

```
aggregate_assay(asy, by, FUN)
```

**Arguments**

asy	A <code>BumpyMatrix</code> object.
by	Character vector of the nested fields to aggregate by.
FUN	A function to use to aggregate the data.

**Value**

A BumpyMatrix object aggregated by FUN.

**Examples**

```
mae <- get_synthetic_data("finalMAE_small")
se <- mae[[1]]
assay <- SummarizedExperiment::assay(se)
aggregate_assay(assay, FUN = mean, by = c("Barcode"))
```

---

apply\_bumpy\_function *Apply a function to every element of a bumpy matrix.*

---

**Description**

Apply a user-specified function to every element of a bumpy matrix.

**Usage**

```
apply_bumpy_function(
  se,
  FUN,
  req_assay_name,
  out_assay_name,
  parallelize = FALSE,
  ...
)
```

**Arguments**

**se** A SummarizedExperiment object with bumpy matrices.

**FUN** A function that will be applied to each element of the matrix in assay req\_assay\_name. Output of the function must return a data.table.

**req\_assay\_name** String of the assay name in the se that the FUN will act on.

**out\_assay\_name** String of the assay name that will contain the results of the applied function.

**parallelize** Logical indicating whether or not to parallelize the computation.

**...** Additional args to be passed to teh FUN.

**Value**

The original se object with a new assay, out\_assay\_name.

**Examples**

```
mae <- get_synthetic_data("finalMAE_small.qs")
se <- mae[[1]]
FUN <- function(x) {
  data.table::data.table(Concentration = x$Concentration, CorrectedReadout = x$CorrectedReadout)
}
apply_bumpy_function(
  se,
  FUN = FUN,
  req_assay_name = "RawTreated",
  out_assay_name = "CorrectedReadout"
)
```

---

assert\_choices

*assert\_choices*

---

**Description**

assert choices

**Usage**

```
assert_choices(x, choices, ...)
```

**Arguments**

x	charvec expected subset
choices	charvec reference set
...	Additional arguments to pass to <code>checkmate::test_choice</code>

**Value**

NULL

**Examples**

```
assert_choices("x", c("x", "y"))
```

---

average\_biological\_replicates\_dt  
*Average biological replicates.*

---

### Description

Average biological replicates on the data table side.

### Usage

```
average_biological_replicates_dt(  
  dt,  
  var,  
  pidfs = get_prettified_identifiers(),  
  fixed = TRUE,  
  geometric_average_fields = get_header("metric_average_fields")$geometric_mean  
)
```

### Arguments

dt	data.table with Metric data
var	String representing additional metadata of replicates
pidfs	list of prettified identifiers
fixed	Flag should be add fix for -Inf in geometric mean.
geometric_average_fields	Character vector of column names in dt to take the geometric average of.

### Value

data.table without replicates

### Examples

```
dt <- data.table::data.table(a = c(1:10, 1),  
  b = c(rep("drugA", 10), rep("drugB", 1)))  
average_biological_replicates_dt(dt, var = "a")
```



---

cap_xc50	<i>Cap XC50 value.</i>
----------	------------------------

---

### Description

Set IC50/GR50 value to Inf or -Inf based on upper and lower limits.

### Usage

```
cap_xc50(xc50, max_conc, min_conc = NA, capping_fold = 5)
```

### Arguments

xc50	Numeric value of the IC50/GR50 to cap.
max_conc	Numeric value of the highest concentration in a dose series used to calculate the xc50.
min_conc	Numeric value of the lowest concentration in a dose series used to calculate the xc50. If NA (default), using max_conc/1e5 instead.
capping_fold	Integer value of the fold number to use for capping. Defaults to 5.

### Details

Note: xc50 and max\_conc should share the same units. Ideally, the lower\_cap should be based on the lowest tested concentration. However, since we don't record that, it is set 5 orders of magnitude below the highest dose.

### Value

Capped IC50/GR50 value.

### Examples

```
cap_xc50(xc50 = 1, max_conc = 2)
cap_xc50(xc50 = 2, max_conc = 5, min_conc = 1)
cap_xc50(xc50 = 26, max_conc = 5, capping_fold = 5)
```

---

`convert_colData_to_json`*Convert colData to JSON*

---

### Description

Convert colData to JSON format for elasticsearch indexing.

### Usage

```
convert_colData_to_json(  
  cdata,  
  identifiers,  
  req_cols = c("cellline", "cellline_name", "cellline_tissue", "cellline_ref_div_time")  
)
```

### Arguments

<code>cdata</code>	data.table of colData.
<code>identifiers</code>	charvec with identifiers
<code>req_cols</code>	charvec required columns

### Details

Standardizes the cdata to common schema fields and tidies formatting to be conducive to joining with other JSON responses.

### Value

JSON string capturing the cdata.

### Examples

```
cdata <- data.table::data.table(  
  mycellline = letters,  
  mycelllinename = letters,  
  mycelllinetissue = letters,  
  cellline_ref_div_time = "cellline_ref_div_time")  
identifiers <- list(cellline = "mycellline",  
  cellline_name = "mycelllinename",  
  cellline_ref_div_time = "cellline_ref_div_time",  
  cellline_tissue = "mycelllinetissue")  
convert_colData_to_json(cdata, identifiers)
```

---

`convert_combo_data_to_dt`

*convert combo assays from SummarizedExperiments to the list of data.tables*

---

**Description**

convert combo assays from SummarizedExperiments to the list of data.tables

**Usage**

```
convert_combo_data_to_dt(  
  se,  
  c_assays = get_combo_assay_names(),  
  normalization_type = c("RV", "GR"),  
  prettify = TRUE  
)
```

**Arguments**

<code>se</code>	SummarizedExperiment object with dose-response data
<code>c_assays</code>	charvec of combo assays to be used
<code>normalization_type</code>	charvec of normalization_types expected in the data
<code>prettify</code>	boolean flag indicating whether or not to prettify the colnames of the returned data

**Value**

list of data.table(s) with combo data

**Author(s)**

Arkadiusz Gładki <arkadiusz.gladki@contractors.roche.com>

**Examples**

```
mae <- get_synthetic_data("finalMAE_combo_matrix_small.qs")  
convert_combo_data_to_dt(mae[[1]])
```

---

```
convert_combo_field_to_assay
    get combo assay names based on the field name
```

---

**Description**

get combo assay names based on the field name

**Usage**

```
convert_combo_field_to_assay(field)
```

**Arguments**

field                   String containing name of the field for which the assay name should be returned

**Value**

charvec

**Examples**

```
convert_combo_field_to_assay("hsa_score")
```

---

```
convert_mae_assay_to_dt
    Convert a MultiAssayExperiment assay to a long data.table
```

---

**Description**

Convert an assay within a [SummarizedExperiment](#) object in a MultiAssayExperiment to a long data.table.

**Usage**

```
convert_mae_assay_to_dt(
  mae,
  assay_name,
  experiment_name = NULL,
  include_metadata = TRUE,
  retain_nested_rownames = FALSE,
  wide_structure = FALSE
)
```

## Arguments

mae	A <a href="#">MultiAssayExperiment</a> object holding experiments with raw and/or processed dose-response data in its assays.
assay_name	String of name of the assay to transform within an experiment of the mae.
experiment_name	String of name of the experiment in mae whose assay_name should be converted. Defaults to NULL to indicate to convert assay in all experiments into one data.table object.
include_metadata	Boolean indicating whether or not to include rowData() and colData() in the returned data.table. Defaults to TRUE.
retain_nested_rownames	Boolean indicating whether or not to retain the rownames nested within a BumpyMatrix assay. Defaults to FALSE. If the assay_name is not of the BumpyMatrix class, this argument's value is ignored. If TRUE, the resulting column in the data.table will be named as "<assay_name>_rownames".
wide_structure	Boolean indicating whether or not to transform data.table into wide format. wide_structure = TRUE requires retain_nested_rownames = TRUE however that will be validated in convert_se_assay_to_dt function

## Details

NOTE: to extract information about 'Control' data, simply call the function with the name of the assay holding data on controls.

## Value

data.table representation of the data in assay\_name.

## Author(s)

Bartosz Czech [bartosz.czech@contractors.roche.com](mailto:bartosz.czech@contractors.roche.com)

## See Also

flatten convert\_se\_assay\_to\_dt

## Examples

```
mae <- get_synthetic_data("finalMAE_small")
convert_mae_assay_to_dt(mae, "Metrics")
```

---

convert\_mae\_to\_json    *Create JSON document.*

---

**Description**

Convert a MultiAssayExperiment object to a JSON document.

**Usage**

```
convert_mae_to_json(mae, with_experiments = TRUE)
```

**Arguments**

mae                    SummarizedExperiment object.  
with\_experiments      logical convert experiment metadata as well?

**Value**

String representation of a JSON document.

**Examples**

```
mae <- get_synthetic_data("finalMAE_small")  
convert_mae_to_json(mae)  
convert_mae_to_json(mae, with_experiments = FALSE)
```

---

convert\_metadata\_to\_json  
                          *Convert experiment metadata to JSON format for elasticsearch indexing.*

---

**Description**

Convert experiment metadata to JSON format for elasticsearch indexing.

**Usage**

```
convert_metadata_to_json(se)
```

**Arguments**

se                    SummarizedExperiment object.

**Value**

JSON string capturing experiment metadata.

**Examples**

```
md <- list(title = "my awesome experiment",
  description = "description of experiment",
  sources = list(list(name = "GeneData_Screener", id = "QCS-12345")))
se <- SummarizedExperiment::SummarizedExperiment(metadata = md)
convert_metadata_to_json(se)
```

---

convert\_rowData\_to\_json

*Convert rowData to JSON*

---

**Description**

Convert rowData to JSON format for elasticsearch indexing.

**Usage**

```
convert_rowData_to_json(
  rdata,
  identifiers,
  req_cols = c("drug", "drug_name", "drug_moa", "duration")
)
```

**Arguments**

rdata	data.table of rowData.
identifiers	charvec with identifiers
req_cols	charvec required columns

**Details**

Standardizes the rdata to common schema fields and tidies formatting to be conducive to joining with other JSON responses.

**Value**

JSON string capturing the rdata.

**Examples**

```
rdata <- data.table::data.table(
  mydrug = letters,
  mydrugname = letters,
  mydrugmoa = letters,
  Duration = 1)
identifiers <- list(drug = "mydrug", drug_name = "mydrugname", drug_moa = "mydrugmoa",
  duration = "Duration")
convert_rowData_to_json(rdata, identifiers)
```

---

```
convert_se_assay_to_custom_dt
```

*Convert a SummarizedExperiment assay to a long data.table and conduct some post processing steps*

---

**Description**

Convert an assay within a SummarizedExperiment object to a long data.table. Then conduct some post processing steps.

**Usage**

```
convert_se_assay_to_custom_dt(se, assay_name, output_table = NULL)
```

**Arguments**

se	A SummarizedExperiment object holding raw and/or processed dose-response data in its assays.
assay_name	String of name of the assay to transform within the se.
output_table	String of type name of the output data.table

**Details**

Current strategy is per-assay specific.

1. combo assays: conversion to data.table only (with wide\_structure = FALSE)
2. 'Metrics' assay can be converted to three types of outputs:
  - Metrics\_initial (conversion to data.table only, with wide\_structure = FALSE)
  - Metrics\_raw: same as Metrics\_initial followed by:
    - fix for 'EC50' and 'Metrics\_rownames'
    - flatten
    - prettifying and dropping excess variables
  - Metrics (same as Metrics\_raw + capVals)



1. 'Normalization' and 'Averaged' assay:

- conversion to data.table (with wide\_structure = TRUE)
- prettifying and dropping excess variables

NOTE: to extract information about 'Control' data, simply call the function with the name of the assay holding data on controls. To extract the reference data in to same format as 'Averaged' use `convert_se_ref_assay_to_dt`.

### Value

data.table representation of the data in assay\_name with added information from colData.

### See Also

`convert_se_assay_to_dt`

### Examples

```
mae <- get_synthetic_data("finalMAE_small")
se <- mae[[1]]
convert_se_assay_to_custom_dt(se, "Metrics")
convert_se_assay_to_custom_dt(se, "Metrics", output_table = "Metrics_raw")
convert_se_assay_to_custom_dt(se, "Metrics", output_table = "Metrics_initial")
convert_se_assay_to_custom_dt(se, "Averaged")
```

---

`convert_se_assay_to_dt`

*Convert a SummarizedExperiment assay to a long data.table*

---

### Description

Convert an assay within a [SummarizedExperiment](#) object to a long data.table.

### Usage

```
convert_se_assay_to_dt(
  se,
  assay_name,
  include_metadata = TRUE,
  retain_nested_rownames = FALSE,
  wide_structure = FALSE
)
```

**Arguments**

se	A <a href="#">SummarizedExperiment</a> object holding raw and/or processed dose-response data in its assays.
assay_name	String of name of the assay to transform within the se.
include_metadata	Boolean indicating whether or not to include rowData(se) and colData(se) in the returned data.table. Defaults to TRUE.
retain_nested_rownames	Boolean indicating whether or not to retain the rownames nested within a BumpyMatrix assay. Defaults to FALSE. If the assay_name is not of the BumpyMatrix class, this argument's value is ignored. If TRUE, the resulting column in the data.table will be named as "<assay_name>_rownames".
wide_structure	Boolean indicating whether or not to transform data.table into wide format. wide_structure = TRUE requires retain_nested_rownames = TRUE.

**Details**

NOTE: to extract information about 'Control' data, simply call the function with the name of the assay holding data on controls. To extract the reference data in to same format as 'Averaged' use `convert_se_ref_assay_to_dt`.

**Value**

data.table representation of the data in assay\_name.

**See Also**

`flatten`

**Examples**

```
mae <- get_synthetic_data("finalMAE_small")
se <- mae[[1]]
convert_se_assay_to_dt(se, "Metrics")
```

---

`convert_se_to_json`      *Convert a SummarizedExperiment object to a JSON document.*

---

**Description**

Convert a SummarizedExperiment object to a JSON document.

**Usage**

```
convert_se_to_json(se)
```

**Arguments**

se SummarizedExperiment object.

**Value**

String representation of a JSON document.

**Examples**

```
md <- list(title = "my awesome experiment",
  description = "description of experiment",
  source = list(name = "GeneData_Screener", id = "QCS-12345"))
rdata <- data.table::data.table(
  mydrug = letters,
  mydrugname = letters,
  mydrugmoa = letters,
  Duration = 1)
cdata <- data.table::data.table(mycellline = letters, mycelllinename = letters,
  mycelllinetissue = letters, cellline_ref_div_time = letters)
identifiers <- list(cellline = "mycellline",
  cellline_name = "mycelllinename",
  cellline_tissue = "mycelllinetissue",
  cellline_ref_div_time = "cellline_ref_div_time",
  drug = "mydrug",
  drug_name = "mydrugname",
  drug_moa = "mydrugmoa",
  duration = "Duration")
se <- SummarizedExperiment::SummarizedExperiment(rowData = rdata,
  colData = cdata)

se <- set_SE_experiment_metadata(se, md)
se <- set_SE_identifiers(se, identifiers)
convert_se_to_json(se)
```

---

define\_matrix\_grid\_positions

*Define matrix grid positions*

---

**Description**

Define matrix grid positions

**Usage**

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

**Arguments**

conc1 drug\_1 concentration  
 conc2 drug\_2 concentration

**Details**

drug\_1 is diluted along the rows as the y-axis and drug\_2 is diluted along the columns and will be the x-axis.

**Value**

list with axis grid positions

**Examples**

```

cl_name <- "cellline_BC"
drug1_name <- "drug_001"
drug2_name <- "drug_026"

se <- get_synthetic_data("combo_matrix_small")[["combination"]]
dt_average <- convert_se_assay_to_dt(se, "Averaged")[normalization_type == "GR"]

ls_axes <- define_matrix_grid_positions(
  dt_average[["Concentration"]], dt_average[["Concentration_2"]])

```

---

demote_fields	<i>Demote a metadata field in the rowData or colData of a SummarizedExperiment object to a nested field of a BumpyMatrix assay.</i>
---------------	---

---

**Description**

Demote a metadata field in the rowData or colData of a SummarizedExperiment object to a nested field of a BumpyMatrix assay.

**Usage**

```
demote_fields(se, fields)
```

**Arguments**

se	A SummarizedExperiment object.
fields	Character vector of metadata fields to demote as nested columns.

**Details**

Revert this operation using promote\_fields.

**Value**

A SummarizedExperiment object with new dimensions resulting from demoting given fields to nested columns.

**See Also**

promote\_fields

**Examples**

```
mae <- get_synthetic_data("finalMAE_small")
se <- mae[[1]]
se <- promote_fields(se, "ReadoutValue", 2)
demote_fields(se, "ReadoutValue")
```

---

df_to_bm_assay	<i>df_to_bm_assay</i>
----------------	-----------------------

---

**Description**

Convert data.table with dose-response data into a BumpyMatrix assay.

**Usage**

```
df_to_bm_assay(data, discard_keys = NULL)
```

**Arguments**

data            data.table with drug-response data  
discard\_keys   a vector of keys that should be discarded

**Details**

The 'assay' is simply a BumpyMatrix object with rownames being the treatment ids, colnames being the ids of the cell lines and values with dose-response data for given cell lines under given conditions.

**Value**

BumpyMatrix object

**Examples**

```
df_to_bm_assay(data.table::data.table(Gnumber = 2, clid = "A"))
```

---

extend\_normalization\_type\_name  
*extend abbreviated normalization type*

---

**Description**

extend abbreviated normalization type

**Usage**

extend\_normalization\_type\_name(x)

**Arguments**

x                    string with normalization type

**Value**

string

**Examples**

```
extend_normalization_type_name("GR")
```

---

fit_curves	<i>Fit curves</i>
------------	-------------------

---

**Description**

Fit GR and RV curves from a data.table.

**Usage**

```
fit_curves(
  df_,
  series_identifiers,
  e_0 = 1,
  GR_0 = 1,
  n_point_cutoff = 4,
  range_conc = c(0.005, 5),
  force_fit = FALSE,
  pcutoff = 0.05,
  cap = 0.1,
  normalization_type = c("GR", "RV")
)
```

**Arguments**

<code>df_</code>	data.table containing data to fit. See details.
<code>series_identifiers</code>	character vector of the column names in data.table whose combination represents a unique series for which to fit curves.
<code>e_0</code>	numeric value representing the $x_0$ value for the RV curve. Defaults to 1.
<code>GR_0</code>	numeric value representing the $x_0$ value for the GR curve. Defaults to 1.
<code>n_point_cutoff</code>	integer of how many points should be considered the minimum required to try to fit a curve. Defaults to 4.
<code>range_conc</code>	numeric vector of length 2 indicating the lower and upper concentration ranges. Defaults to <code>c(5e-3, 5)</code> . See details.
<code>force_fit</code>	boolean indicating whether or not to force a constant fit. Defaults to FALSE.
<code>p cutoff</code>	numeric of pvalue significance threshold above or equal to which to use a constant fit. Defaults to <code>0.05</code> .
<code>cap</code>	numeric value capping norm_values to stay below $(x_0 + cap)$ . Defaults to <code>0.1</code> .
<code>normalization_type</code>	character vector of types of curves to fit. Defaults to <code>c("GR", "RV")</code> .

**Details**

The `df_` expects the following columns:

- RelativeViability normalized relative viability values (if `normalization_type` includes "RV")
- GRvalue normalized GR values (if `normalization_type` includes "GR")

The `range_conc` is used to calculate the `x_AOC_range` statistic. The purpose of this statistic is to enable comparison across different experiments with slightly different concentration ranges.

**Value**

data.table of fit parameters as specified by the `normalization_type`.

**Examples**

```
df_ <- data.table::data.table(Concentration = c(0.001, 0.00316227766016838,
0.01, 0.0316227766016838),
x_std = c(0.1, 0.1, 0.1, 0.1), normalization_types = c("RV", "RV", "RV", "RV"),
x = c(0.9999964000144, 0.999964001439942, 0.999640143942423, 0.996414342629482))

fit_curves(df_, "Concentration", normalization_type = "RV")
```

---

flatten	<i>Flatten a table</i>
---------	------------------------

---

### Description

Flatten a stacked table into a wide format.

### Usage

```
flatten(tbl, groups, wide_cols, sep = "_")
```

### Arguments

tbl	table to flatten.
groups	character vector of column names representing unifying groups in expansion.
wide_cols	character vector of column names to flatten.
sep	string representing separator between wide_cols columns, used in column re-naming. Defaults to "_".

### Details

flattened columns will be named with original column names prefixed by wide\_cols columns, concatenated together and separated by sep.

A common use case for this function is when a flattened version of the "Metrics" assay is desired.

### Value

table of flattened data as defined by wide\_cols.

### See Also

`convert_se_assay_to_dt`

### Examples

```
n <- 4
m <- 5
grid <- expand.grid(normalization_type = c("GR", "RV"),
  source = c("GDS", "GDR"))
regrid <- data.table::rbindlist(rep(list(grid), m))
regrid$wide <- seq(m * n)
regrid$id <- rep(LETTERS[1:m], each = n)

groups <- colnames(grid)
wide_cols <- c("wide")

flatten(regrid, groups = groups, wide_cols = wide_cols)
```



---

gen\_synthetic\_data      *gen\_synthetic\_data*

---

**Description**

Function for generating local synthetic data used for unit tests in modules

**Usage**

```
gen_synthetic_data(m = 1, n = 5)
```

**Arguments**

m	number of drugs
n	number of records

**Value**

list with drugs, cell\_lines, raw\_data and assay\_data

**Examples**

```
gen_synthetic_data()
```

---

get\_additional\_variables

*Identify and return additional variables in list of dt*

---

**Description**

Identify and return additional variables in list of dt

**Usage**

```
get_additional_variables(  
  dt_list,  
  pidfs = get_prettified_identifiers(),  
  unique = FALSE  
)
```

**Arguments**

dt_list	list of data.table or data.table containing additional variables
pidfs	list of prettified identifiers
unique	logical flag indicating if all variables should be returned or only those containing more than one unique value

**Value**

vector of variable names with additional variables

**Examples**

```
dt <- data.table::data.table(  
  Gnumber = seq_len(10),  
  Concentration = runif(10),  
  Ligand = c(rep(0.5, 5), rep(0, 5))  
)  
get_additional_variables(dt)
```

---

get_assay_names	<i>get assay names of the given se/dataset fetch the data from the se if provided as metadata use predefined values from get_env_assay_names otherwise</i>
-----------------	--

---

**Description**

get assay names of the given se/dataset fetch the data from the se if provided as metadata use predefined values from get\_env\_assay\_names otherwise

**Usage**

```
get_assay_names(se = NULL, ...)
```

**Arguments**

se	SummarizedExperiment or NULL
...	Additional arguments to pass to get_env_assay_names.

**Value**

charvec

**Author(s)**

Arkadiusz Gładki <arkadiusz.gladki@contractors.roche.com>

**Examples**

```
get_assay_names()
```

---

get\_combo\_assay\_names *get names of combo assays*

---

**Description**

get names of combo assays

**Usage**

```
get_combo_assay_names(se = NULL, ...)
```

**Arguments**

se	SummarizedExperiment or NULL
...	Additional arguments to pass to get_assay_names.

**Value**

charvec of combo assay names.

**Author(s)**

Arkadiusz Gładki <arkadiusz.gladki@contractors.roche.com>

**Examples**

```
get_combo_assay_names()
```

---

get\_combo\_base\_assay\_names  
*get names of combo base assays*

---

**Description**

get names of combo base assays

**Usage**

```
get_combo_base_assay_names(se = NULL, ...)
```

**Arguments**

se	SummarizedExperiment or NULL
...	Additional arguments to pass to get_combo_assay_names.

**Value**

charvec

**Author(s)**

Arkadiusz Gładki <arkadiusz.gladki@contractors.roche.com>

**Examples**

```
get_combo_base_assay_names()
```

---

```
get_combo_col_settings
```

*Get colorscale data for given combo assay and growth metric*

---

**Description**

Get colorscale data for given combo assay and growth metric

**Usage**

```
get_combo_col_settings(g_metric, assay_type)
```

**Arguments**

`g_metric` growth metric

`assay_type` assay type

**Value**

list with colors, breaks and limits

**Examples**

```
get_combo_col_settings("GR", "excess")
```

---

`get_combo_excess_field_names`  
*get names of combo excess fields*

---

**Description**

get names of combo excess fields

**Usage**

`get_combo_excess_field_names()`

**Value**

charvec

**Examples**

`get_combo_excess_field_names()`

---

`get_combo_score_assay_names`  
*get names of combo score assays*

---

**Description**

get names of combo score assays

**Usage**

`get_combo_score_assay_names(se = NULL, ...)`

**Arguments**

`se` SummarizedExperiment or NULL  
`...` Additional arguments to pass to `get_combo_assay_names`.

**Value**

charvec

**Author(s)**

Arkadiusz Gładki <arkadiusz.gladki@contractors.roche.com>

**Examples**

```
get_combo_score_assay_names()
```

---

```
get_combo_score_field_names
```

*get names of combo score fields*

---

**Description**

get names of combo score fields

**Usage**

```
get_combo_score_field_names()
```

**Value**

charvec

**Examples**

```
get_combo_score_assay_names()
```

---

```
get_default_identifiers
```

*Get gDR default identifiers required for downstream analysis.*

---

**Description**

Get gDR default identifiers required for downstream analysis.

**Usage**

```
get_default_identifiers()
```

**Value**

charvec

**Examples**

```
get_default_identifiers()
```

---

get\_duplicated\_rows *Helper function to find duplicated rows*

---

**Description**

Helper function to find duplicated rows

**Usage**

```
get_duplicated_rows(x, col_names = NULL)
```

**Arguments**

x                    data frame  
col\_names            character vector, columns in which duplication are searched for

**Value**

integer vector

**Examples**

```
dt <- data.table::data.table(a = c(1, 2, 3), b = c(3, 2, 2))  
get_duplicated_rows(dt, "b")
```

---

get\_env\_assay\_names *get default assay names for the specified filters, i.e. set of assay types, assay groups and assay data types*

---

**Description**

get default assay names for the specified filters, i.e. set of assay types, assay groups and assay data types

**Usage**

```
get_env_assay_names(  
  type = NULL,  
  group = NULL,  
  data_type = NULL,  
  prettify = FALSE,  
  simplify = TRUE  
)
```

**Arguments**

type	charvec of assay types
group	charvec of assay groups
data_type	charvec assay of data types
prettify	logical flag, prettify the assay name?
simplify	logical flag, simplify the output? will return single string instead of named vector with single element useful when function is expected to return single element/assay only

**Value**

charvec

**Author(s)**

Arkadiusz Gładki <arkadiusz.gladki@contractors.roche.com>

**Examples**

```
get_env_assay_names()
```

---

get\_expect\_one\_identifiers

*Get identifiers that expect only one value for each identifier.*

---

**Description**

Get identifiers that expect only one value for each identifier.

**Usage**

```
get_expect_one_identifiers()
```

**Value**

charvec

**Examples**

```
get_expect_one_identifiers()
```



---

get\_experiment\_groups *get\_experiment\_groups*

---

**Description**

get experiment groups

**Usage**

```
get_experiment_groups(type = NULL)
```

**Arguments**

type                   String indicating the name of an assay group. Defaults to all experiment groups.

**Value**

list with experiment groups or string (if type not NULL)

**Author(s)**

Arkadiusz Gladki [arkadiusz.gladki@contractors.roche.com](mailto:arkadiusz.gladki@contractors.roche.com)

**Examples**

```
get_experiment_groups()
```

---

get\_identifiers\_dt     *Get descriptions for identifiers*

---

**Description**

Get descriptions for identifiers

**Usage**

```
get_identifiers_dt(k = NULL, get_description = FALSE, get_example = FALSE)
```

**Arguments**

k                        identifier key, string  
get\_description         return descriptions only, boolean  
get\_example             return examples only, boolean

**Value**

named list

**Examples**

```
get_identifiers_dt()
```

---

get_idfs_synonyms	<i>Get gDR synonyms for the identifiers</i>
-------------------	---

---

**Description**

Get gDR synonyms for the identifiers

**Usage**

```
get_idfs_synonyms()
```

**Value**

charvec

**Examples**

```
get_idfs_synonyms()
```

---

get_isobologram_columns	<i>Get isobologram column names</i>
-------------------------	-------------------------------------

---

**Description**

Get isobologram column names

**Usage**

```
get_isobologram_columns(k = NULL, prettify = TRUE)
```

**Arguments**

k	key
prettify	change to upper case and add underscore, iso_level -> Iso_Level

**Value**

character vector of isobologram column names for combination data

**Examples**

```
get_isobologram_columns()  
get_isobologram_columns("iso_level", prettify = TRUE)
```

---

*get\_iso\_colors*      *get\_iso\_colors*

---

**Description**

*get\_iso\_colors*

**Usage**

```
get_iso_colors(normalization_type = c("RV", "GR"))
```

**Arguments**

*normalization\_type*  
charvec *normalization\_types* expected in the data

**Value**

named charvec with iso colors

**Examples**

```
get_iso_colors()
```

---

*get\_MAE\_identifiers*      *get\_MAE\_identifiers*

---

**Description**

get the identifiers of all SE's in the MAE

**Usage**

```
get_MAE_identifiers(mae)
```

**Arguments**

mae                    MultiAssayExperiment

**Value**

named list with identifiers for each SE

**Examples**

```
mae <- get_synthetic_data("finalMAE_small.qs")
get_MAE_identifiers(mae)
```

---

`get_non_empty_assays`    *get\_non\_empty\_assays*

---

**Description**

get non empty assays

**Usage**

```
get_non_empty_assays(mae)
```

**Arguments**

mae                    MultiAssayExperiment object

**Value**

charvec with non-empty experiments

**Author(s)**

Arkadiusz Gladki [arkadiusz.gladki@contractors.roche.com](mailto:arkadiusz.gladki@contractors.roche.com)

**Examples**

```
mae <- get_synthetic_data("finalMAE_small.qs")
get_non_empty_assays(mae)
```

---

`get_optional_coldata_fields`  
*get optional colData fields*

---

**Description**

get optional colData fields

**Usage**

`get_optional_coldata_fields(se)`

**Arguments**

`se` a SummarizedExperiment object with drug-response data generate by gDR pipeline

**Value**

a charvec containing the names of the optional identifiers in the SE colData

---

`get_optional_rowdata_fields`  
*get optional rowData fields*

---

**Description**

get optional rowData fields

**Usage**

`get_optional_rowdata_fields(se)`

**Arguments**

`se` a SummarizedExperiment object with drug-response data generate by gDR pipeline

**Value**

a charvec containing the names of the optional identifiers in the SE rowData

get\_required\_identifiers

*Get identifiers required for downstream analysis.*

---

### **Description**

Get identifiers required for downstream analysis.

### **Usage**

```
get_required_identifiers()
```

### **Value**

charvec

### **Examples**

```
get_required_identifiers()
```

---

get\_settings\_from\_json

*Get settings from JSON file In most common scenario the settings are stored in JSON file to avoid hardcoding*

---

### **Description**

Get settings from JSON file In most common scenario the settings are stored in JSON file to avoid hardcoding

### **Usage**

```
get_settings_from_json(  
    s = NULL,  
    json_path = system.file(package = "gDRutils", "cache.json")  
)
```

### **Arguments**

s                    charvec with setting entry/entries  
json\_path            string with the path to the JSON file

### **Value**

value/values for entry/entries from JSON file

### Examples

```
if (!nchar(system.file(package="gDRutils"))) {  
  get_settings_from_json()  
}
```

---

`get_supported_experiments`  
*get\_supported\_experiments*

---

### Description

get supported experiments

### Usage

```
get_supported_experiments(type = NULL)
```

### Arguments

type                   String indicating the type of experiment

### Value

charvec with supported experiment name(s)

### Author(s)

Arkadiusz Gladki [arkadiusz.gladki@contractors.roche.com](mailto:arkadiusz.gladki@contractors.roche.com)

### Examples

```
get_supported_experiments()
```

---

get\_synthetic\_data      *Get synthetic data from gDRtestData package*

---

**Description**

Get synthetic data from gDRtestData package

**Usage**

```
get_synthetic_data(qs)
```

**Arguments**

qs                      qs filename

**Value**

loaded data

**Examples**

```
get_synthetic_data("finalMAE_small.qs")
```

---

get\_testdata              *get\_testdata*

---

**Description**

Function to obtain data from gDRtestData and prepare for unit tests

**Usage**

```
get_testdata()
```

**Value**

list with drugs, cell\_lines, raw\_data and assay\_data

**Examples**

```
get_testdata()
```



---

`get_testdata_codilution`  
*get\_testdata\_codilution*

---

**Description**

Function to obtain data from gDRtestData and prepare for unit tests

**Usage**

`get_testdata_codilution()`

**Value**

list with `drugs`, `cell_lines`, `raw_data` and `assay_data`

**Examples**

`get_testdata_codilution()`

---

`get_testdata_combo`     *get\_testdata\_combo*

---

**Description**

Function to obtain data from gDRtestData and prepare for unit tests

**Usage**

`get_testdata_combo()`

**Value**

list with `drugs`, `cell_lines`, `raw_data` and `assay_data`

**Examples**

`get_testdata_combo()`

---

has\_single\_codrug\_data

*Has Single Codrug Data*

---

## Description

Has Single Codrug Data

## Usage

```
has_single_codrug_data(  
  cols,  
  prettify_identifiers = TRUE,  
  codrug_identifiers = c("drug_name2", "concentration2")  
)
```

## Arguments

`cols` character vector with the columns of the input data

`prettify_identifiers` logical flag specifying if identifiers are expected to be prettified

`codrug_identifiers` character vector with identifiers for the codrug columns

## Value

logical flag

## Examples

```
has_single_codrug_data("Drug Name")  
has_single_codrug_data(c("Drug Name", "Cell Lines"))  
has_single_codrug_data(c("Drug Name 2", "Concentration 2"))  
has_single_codrug_data(  
  get_prettified_identifiers(  
    c("concentration2", "drug_name2"),  
    simplify = FALSE  
  )  
)
```

---

has\_valid\_codrug\_data *Has Valid Codrug Data*

---

### Description

Has Valid Codrug Data

### Usage

```
has_valid_codrug_data(  
  data,  
  prettify_identifiers = TRUE,  
  codrug_name_identifier = "drug_name2",  
  codrug_conc_identifier = "concentration2"  
)
```

### Arguments

`data` data.table with input data

`prettify_identifiers` logical flag specifying if identifiers are expected to be prettified

`codrug_name_identifier` string with the identifiers for the codrug drug\_name column

`codrug_conc_identifier` string with the identifiers for the codrug concentration column

### Value

logical flag

### Examples

```
dt <-  
  data.table::data.table(  
    "Drug Name" = letters[seq_len(3)],  
    "Concentration" = seq_len(3),  
    "Drug Name 2" = letters[4:6],  
    "Concentration 2" = 4:6  
  )  
has_valid_codrug_data(dt)  
  
dt$`Concentration 2` <- NULL  
has_valid_codrug_data(dt)
```

---

headers	<i>Get or reset headers for one or all header field(s) respectively</i>
---------	---

---

**Description**

Get the expected header(s) for one field or reset all header fields

**Usage**

```
get_header(k = NULL)
```

**Arguments**

k                    string of field (data type) to return headers for

**Details**

If `get_header` is called with no values, the entire available header list is returned.

**Value**

For `get_header` a character vector of headers for field `k`.

**Examples**

```
get_header(k = NULL)
get_header("manifest")
```

---

identifiers	<i>Get, set, or reset identifiers for one or all identifier field(s)</i>
-------------	--

---

**Description**

Get, set, or reset the expected identifier(s) for one or all identifier field(s). Identifiers are used by the `gDR` processing functions to identify which columns in a `data.table` correspond to certain expected fields. Functions of the family `*et_identifier` will look for identifiers from the environment while functions of the family `*et_SE_identifiers` will look for identifiers in the metadata slot of a `SummarizedExperiment` object. See details for expected identifiers and their definitions.

**Usage**

```
get_env_identifiers(k = NULL, simplify = TRUE)
get_prettified_identifiers(k = NULL, simplify = TRUE)
set_env_identifier(k, v)
reset_env_identifiers()
```

## Arguments

k	String corresponding to identifier name.
simplify	Boolean indicating whether output should be simplified.
v	Character vector corresponding to the value for given identifier k.

## Details

Identifiers supported by the gDR suite include:

- "barcode": String of column name containing barcode metadata
- "cellline": String of column name containing unique, machine-readable cell line identifiers
- "cellline\_name": String of column name containing human-friendly cell line names
- "cellline\_tissue": String of column name containing metadata on cell line tissue type
- "cellline\_ref\_div\_time": String of column name containing reference division time for cell lines
- "cellline\_parental\_identifier": String of column name containing unique, machine-readable parental cell line identifiers. Used in the case of derived or engineered cell lines.
- "drug": String of column name containing unique, machine-readable drug identifiers
- "drug\_name": String of column name containing human-friendly drug names
- "drug\_moa": String of column name containing metadata for drug mode of action
- "duration": String of column name containing metadata on duration that cells were treated (in hours)
- "template": String of column name containing template metadata
- "untreated\_tag": Character vector of entries that identify control, untreated wells
- "well\_position": Character vector of column names containing metadata on well positions on a plate

## Value

For any setting or resetting functionality, a NULL invisibly. For `get_env_identifiers` a character vector of identifiers for field k. For functions called with no arguments, the entire available identifier list is returned.

list or charvec depends on unify param

list or charvec depends on unify param

NULL

NULL

## Examples

```
get_env_identifiers("duration") # "Duration"
```

---

```
identify_unique_se_metadata_fields
```

*Identify unique metadata fields from a list of SummarizedExperiments*

---

**Description**

Identify unique metadata fields from a list of SummarizedExperiments

**Usage**

```
identify_unique_se_metadata_fields(SElist)
```

**Arguments**

SElist            named list of SummarizedExperiments

**Value**

character vector of unique names of metadata

**Examples**

```
mae <- get_synthetic_data("finalMAE_small")
se <- mae[[1]]
SElist <- list(
  se,
  se
)
identify_unique_se_metadata_fields(SElist)
```

---

```
is_any_exp_empty        is_any_exp_empty
```

---

**Description**

check if any experiment is empty

**Usage**

```
is_any_exp_empty(mae)
```

**Arguments**

mae                MultiAssayExperiment object

**Value**

logical

**Author(s)**

Arkadiusz Gladki [arkadiusz.gladki@contractors.roche.com](mailto:arkadiusz.gladki@contractors.roche.com)

**Examples**

```
mae <- get_synthetic_data("finalMAE_small.qs")
is_any_exp_empty(mae)
```

---

is_combo_data	<i>Checks if se is combo dataset.</i>
---------------	---------------------------------------

---

**Description**

Checks if se is combo dataset.

**Usage**

```
is_combo_data(se)
```

**Arguments**

se SummarizedExperiment

**Value**

logical

**Examples**

```
se <- get_synthetic_data("combo_matrix")[[1]]
is_combo_data(se)
se <- get_synthetic_data("combo_matrix")[[2]]
is_combo_data(se)
se <- get_synthetic_data("small")[[1]]
is_combo_data(se)
```

---

<i>is_exp_empty</i>	<i>is_exp_empty</i>
---------------------	---------------------

---

**Description**

check if experiment (SE) is empty

**Usage**

```
is_exp_empty(exp)
```

**Arguments**

exp                    [SummarizedExperiment](#) object.

**Value**

logical

**Author(s)**

Arkadiusz Gladki [arkadiusz.gladki@contractors.roche.com](mailto:arkadiusz.gladki@contractors.roche.com)

**Examples**

```
mae <- get_synthetic_data("finalMAE_small.qs")
se <- mae[[1]]
is_exp_empty(se)
```

---

<i>is_mae_empty</i>	<i>is_mae_empty</i>
---------------------	---------------------

---

**Description**

check if all mae experiments are empty

**Usage**

```
is_mae_empty(mae)
```

**Arguments**

mae                    MultiAssayExperiment object



**Value**

logical

**Author(s)**Arkadiusz Gladki [arkadiusz.gladki@contractors.roche.com](mailto:arkadiusz.gladki@contractors.roche.com)**Examples**

```
mae <- get_synthetic_data("finalMAE_small.qs")
is_mae_empty(mae)
```

logisticFit

*Logistic fit***Description**

Fit a logistic curve to drug response data.

**Usage**

```
logisticFit(
  concs,
  norm_values,
  std_norm_values = NA,
  x_0 = 1,
  priors = NULL,
  lower = NULL,
  range_conc = c(0.005, 5),
  force_fit = FALSE,
  pcutoff = 0.05,
  cap = 0.1,
  n_point_cutoff = 4,
  capping_fold = 5
)
```

**Arguments**

concs	concentrations that have not been transformed into log space.
norm_values	normalized response values (Untreated = 1).
std_norm_values	std of values.
x_0	upper limit. Defaults to 1. For co-treatments, this value should be set to NA.
priors	numeric vector containing starting values for all. mean parameters in the model. Overrides any self starter function.

lower	numeric vector of lower limits for all parameters in a 4-param model.
range_conc	range of concentration for calculating AOC_range.
force_fit	boolean indicating whether or not to force a parameter-based fit.
p cutoff	numeric of pvalue significance threshold above or equal to which to use a constant fit.
cap	numeric value capping norm_values to stay below ( $x_0 + \text{cap}$ ).
n_point_cutoff	integer indicating number of unique concentrations required to fit curve.
capping_fold	Integer value of the fold number to use for capping IC50/GR50. Default is 5.

### Details

Implementation of the genedata approach for curve fit: [#nolint](https://screener.genedata.com/documentation/display/DOC15/Business+Response+Curve+Fitting+Model+Selection+and+Fit+Validity)

The output parameter names correspond to the following definitions:

**x\_mean** The mean of a given dose-response metric

**x\_AOC\_range** The range of the area over the curve

**x\_AOC** The area over the GR curve or, respectively, under the relative cell count curve, averaged over the range of concentration values

**xc50** The concentration at which the effect reaches a value of 0.5 based on interpolation of the fitted curve

**x\_max** The maximum effect of the drug

**ec50** The drug concentration at half-maximal effect

**x\_inf** The asymptotic value of the sigmoidal fit to the dose-response data as concentration goes to infinity

**x\_0** The asymptotic metric value corresponding to a concentration of 0 for the primary drug

**h** The hill coefficient of the fitted curve, which reflects how steep the dose-response curve is

**r2** The goodness of the fit

**x\_sd\_avg** The standard deviation of GR/IC

**fit\_type** This will be given by one of the following:

- "DRC4pHillFitModel" Successfully fit with a 4-parameter model
- "DRC3pHillFitModelFixS0" Successfully fit with a 3-parameter model
- "DRCConstantFitResult" Successfully fit with a constant fit
- "DRCTooFewPointsToFit" Not enough points to run a fit
- "DRCInvalidFitResult" Fit was attempted but failed

**maxlog10Concentration** The highest log10 concentration

**N\_conc** Number of unique concentrations

### Value

data.table with metrics and fit parameters.

**Examples**

```
logisticFit(  
  c(0.001, 0.00316227766016838, 0.01, 0.0316227766016838),  
  c(0.9999964000144, 0.999964001439942, 0.999640143942423, 0.996414342629482),  
  rep(0.1, 4),  
  priors = c(2, 0.4, 1, 0.00658113883008419)  
)
```

---

loop	<i>Lapply or bplapply.</i>
------	----------------------------

---

**Description**

Lapply or bplapply.

**Usage**

```
loop(x, FUN, parallelize = TRUE, ...)
```

**Arguments**

x	Vector (atomic or list) or an ‘expression’ object. Other objects (including classed objects) will be coerced by ‘base::as.list’.
FUN	A user-defined function.
parallelize	Logical indicating whether or not to parallelize the computation. Defaults to TRUE.
...	optional argument passed to <a href="#">bplapply</a> if parallelize == TRUE, else to <a href="#">lapply</a> .

**Value**

List containing output of FUN applied to every element in x.

**Examples**

```
loop(list(c(1,2), c(2,3)), sum, parallelize = FALSE)
```

---

`MAEapply`*Lapply through all the experiments in MultiAssayExperiment object*

---

**Description**

Lapply through all the experiments in MultiAssayExperiment object

**Usage**

```
MAEapply(mae, FUN, unify = FALSE, ...)
```

**Arguments**

<code>mae</code>	MultiAssayExperiment object
<code>FUN</code>	function that should be applied on each experiment of MultiAssayExperiment object
<code>unify</code>	logical indicating if the output should be a unlisted object of unique values across all the experiments
<code>...</code>	Additional args to be passed to teh FUN.

**Value**

list or vector depends on unify param

**Author(s)**

Bartosz Czech [bartosz.czech@contractors.roche.com](mailto:bartosz.czech@contractors.roche.com)

**Examples**

```
mae <- get_synthetic_data("finalMAE_small.qs")
MAEapply(mae, SummarizedExperiment::assayNames)
```

---

`mcolData`*mcolData*

---

**Description**

get colData of all experiments

**Usage**

```
mcolData(mae)
```

**Arguments**

mae                    MultiAssayExperiment object

**Value**

data.table with all-experiments colData

**Author(s)**

Arkadiusz Gladki [arkadiusz.gladki@contractors.roche.com](mailto:arkadiusz.gladki@contractors.roche.com)

**Examples**

```
mae <- get_synthetic_data("finalMAE_small.qs")
mcolData(mae)
```

---

merge_assay	<i>Merge assay data</i>
-------------	-------------------------

---

**Description**

Merge assay data

**Usage**

```
merge_assay(  
  SElist,  
  assay_name,  
  additional_col_name = "data_source",  
  discard_keys = NULL  
)
```

**Arguments**

SElist                named list of Summarized Experiments

assay\_name           name of the assay that should be extracted and merged

additional\_col\_name       string of column name that will be added to assay data for the distinction of possible duplicated metrics that can arise from multiple projects

discard\_keys        character vector of string that will be discarded during creating BumpyMatrix object

**Value**

BumpyMatrix or list with data.table + BumpyMatrix

**Examples**

```
mae <- get_synthetic_data("finalMAE_combo_2dose_nonoise")
listSE <- list(
  combo1 = mae[[1]],
  sa = mae[[2]]
)
merge_assay(listSE, "Normalized")
```

---

merge_metadata	<i>Merge metadata</i>
----------------	-----------------------

---

**Description**

Merge metadata

**Usage**

```
merge_metadata(SElist, metadata_fields)
```

**Arguments**

SElist            named list of SummarizedExperiments  
metadata\_fields        vector of metadata names that will be merged

**Value**

list of merged metadata

**Examples**

```
mae <- get_synthetic_data("finalMAE_small")
se <- mae[[1]]
listSE <- list(
  se,
  se
)
metadata_fields <- identify_unique_se_metadata_fields(listSE)
merge_metadata(listSE, metadata_fields)
```

---

merge_SE	<i>Merge multiple Summarized Experiments</i>
----------	--

---

**Description**

Merge multiple Summarized Experiments

**Usage**

```
merge_SE(
  SElist,
  additional_col_name = "data_source",
  discard_keys = c("normalization_type", "fit_source", "record_id", "swap_sa",
    "control_type")
)
```

**Arguments**

SElist	named list of Summarized Experiments
additional_col_name	string with the name of the column that will be added to assay data for the distinction of possible duplicated metrics that can arise from multiple projects
discard_keys	character vector of string that will be discarded during creating BumpyMatrix object

**Value**

merged SummarizedExperiment object

**Examples**

```
se1 <- get_synthetic_data("finalMAE_small")[[1]]
merge_SE(list(se1 = se1, se2 = se1))
```

---

modifyData	<i>modify assay with additional data</i>
------------	--

---

**Description**

Reduce dimensionality of an assay by dropping extra data or combining variables.

**Usage**

```
modifyData(x, ...)  
  
## S3 method for class 'drug_name2'  
modifyData(x, option, keep, ...)  
  
## S3 method for class 'data_source'  
modifyData(x, option, keep, ...)  
  
## Default S3 method:  
modifyData(x, option, keep, ...)
```

**Arguments**

x	a data.table containing an assay
...	additional arguments passed to methods
option	character string specifying the action to be taken, see Details
keep	character string specifying the value of the active variable that will be kept

**Details**

If an assay extracted from a SummarizedExperiment contains additional information, i.e. factors beyond DrugName and CellLineName, that information will be treated in one of three ways, depending on the value of option:

- drop: Some information will be discarded and only one value of the additional variable (chosen by the user) will be kept.
- toDrug: The information is pasted together with the primary drug name. All observations are kept.
- toCellLine: As above, but pasting is done with cell line name.

Depending on the type of additional information, the exact details will differ. This is handled in the app by adding special classes to the data tables and dispatching to S3 methods.

Following modification, the additional columns are discarded.

**Value**

modified object

**Methods (by class)**

- modifyData(drug\_name2): includes the name and concentration of the second drug
- modifyData(data\_source): includes the data source
- modifyData(default): includes the name of other additional variables



**Examples**

```
dt <- data.table::data.table(a = as.character(1:10), b = "data")
dt <- addClass(dt, "a")
modifyData(dt, "average", keep = "b")
```

---

mrowData

*mrowData*

---

**Description**

get rowData of all experiments

**Usage**

```
mrowData(mae)
```

**Arguments**

mae                      MultiAssayExperiment object

**Value**

data.table with all-experiments rowData

**Author(s)**

Arkadiusz Gladki [arkadiusz.gladki@contractors.roche.com](mailto:arkadiusz.gladki@contractors.roche.com)

**Examples**

```
mae <- get_synthetic_data("finalMAE_small.qs")
mrowData(mae)
```

---

predict\_conc\_from\_efficacy

*Predict a concentration for a given efficacy with fit parameters.*

---

**Description**

Predict a concentration for a given efficacy with fit parameters.

**Usage**

```
predict_conc_from_efficacy(efficacy, x_inf, x_0, ec50, h)
```

**Arguments**

<code>efficacy</code>	Numeric vector representing efficacies to predict concentrations for.
<code>x_inf</code>	Numeric vector representing the asymptotic value of the sigmoidal fit to the dose-response data as concentration goes to infinity.
<code>x_0</code>	Numeric vector representing the asymptotic metric value corresponding to a concentration of 0 for the primary drug.
<code>ec50</code>	Numeric vector representing the drug concentration at half-maximal effect.
<code>h</code>	Numeric vector representing the hill coefficient of the fitted curve, which reflects how steep

**Details**

The inverse of this function is `predict_efficacy_from_conc`.

**Value**

Numeric vector representing predicted concentrations from given efficacies and fit parameters.

**See Also**

`predict_efficacy_from_conc.calculate_x50`

**Examples**

```
predict_conc_from_efficacy(efficacy = c(1, 1.5), x_inf = 0.1, x_0 = 1, ec50 = 0.5, h = 2)
```

---

`predict_efficacy_from_conc`

*Predict efficacy values given fit parameters and a concentration.*

---

**Description**

Predict efficacy values given fit parameters and a concentration.

**Usage**

```
predict_efficacy_from_conc(c, x_inf, x_0, ec50, h)
```

**Arguments**

c	Numeric vector representing concentrations to predict efficacies for.
x_inf	Numeric vector representing the asymptotic value of the sigmoidal fit to the dose-response data as concentration goes to infinity.
x_0	Numeric vector representing the asymptotic metric value corresponding to a concentration of 0 for the primary drug.
ec50	Numeric vector representing the drug concentration at half-maximal effect.
h	Numeric vector representing the hill coefficient of the fitted curve, which reflects how steep the dose-response curve is.

**Details**

The inverse of this function is `predict_conc_from_efficacy`.

**Value**

Numeric vector representing predicted efficacies from given concentrations and fit parameters.

**See Also**

`predict_conc_from_efficacy`

**Examples**

```
predict_efficacy_from_conc(c = 1, x_inf = 0.1, x_0 = 1, ec50 = 0.5, h = 2)
```

---

`prettify_flat_metrics` *Prettify metric names in flat 'Metrics' assay*

---

**Description**

Map existing column names of a flattened 'Metrics' assay to prettified names.

**Usage**

```
prettify_flat_metrics(  
  x,  
  human_readable = FALSE,  
  normalization_type = c("GR", "RV")  
)
```

**Arguments**

`x` character vector of names to prettify.

`human_readable` boolean indicating whether or not to return column names in human readable format. Defaults to FALSE.

`normalization_type` character vector with a specified normalization type. Defaults to `c("GR", "RV")`.

**Details**

A common use case for this function is to prettify column names from a flattened version of the "Metrics" assay. Mode "human\_readable" = TRUE is often used for prettification in the context of front-end applications, whereas "human\_readable" = FALSE is often used for prettification in the context of the command line.

**Value**

character vector of prettified names.

**Examples**

```
x <- c("CellLineName", "Tissue", "Primary Tissue", "GR_gDR_x_mean", "GR_gDR_xc50", "RV_GDS_x_mean")
prettify_flat_metrics(x, human_readable = FALSE)
```

---

promote_fields	<i>Promote a nested field to be represented as a metadata field of the SummarizedExperiment as either the rowData or colData.</i>
----------------	---

---

**Description**

Promote a nested field to be represented as a metadata field of the SummarizedExperiment as either the rowData or colData.

**Usage**

```
promote_fields(se, fields, MARGIN = c(1, 2))
```

**Arguments**

`se` SummarizedExperiment object.

`fields` Character vector of nested fields in a BumpyMatrix object to promote to metadata fields of a se.

`MARGIN` Numeric of values 1 or 2 indicating whether to promote fields to rows or columns respectively.

**Details**

Revert this operation using `demote_fields`.

**Value**

A `SummarizedExperiment` object with new dimensions resulting from promoting given fields.

**See Also**

`demote_fields`

**Examples**

```
mae <- get_synthetic_data("finalMAE_small")
se <- mae[[1]]
se <- promote_fields(se, "ReadoutValue", 2)
```

---

<code>refine_coldata</code>	<i>refine colData</i>
-----------------------------	-----------------------

---

**Description**

current improvements done on the `colData` as a standardization step:

- set default value for optional `colData` fields

**Usage**

```
refine_coldata(cd, se, default_v = "Undefined")
```

**Arguments**

<code>cd</code>	DataFrame with <code>colData</code>
<code>se</code>	a <code>SummarizedExperiment</code> object with drug-response data generate by gDR pipeline
<code>default_v</code>	string with default value for optional columns in <code>colData</code>

**Value**

refined `colData`

**Examples**

```
mae <- get_synthetic_data("finalMAE_small.qs")
refine_coldata(SummarizedExperiment::colData(mae[[1]]), mae[[1]])
```

---

refine_rowdata	<i>refine rowData</i>
----------------	-----------------------

---

**Description**

current improvements done on the rowData as a standardization step:

- set default value for optional rowData fields

**Usage**

```
refine_rowdata(rd, se, default_v = "Undefined")
```

**Arguments**

rd	DataFrame with rowData
se	a SummarizedExperiment object with drug-response data generate by gDR pipeline
default_v	string with default value for optional columns in rowData

**Value**

refined rowData

**Examples**

```
mae <- get_synthetic_data("finalMAE_small.qs")
refine_rowdata(SummarizedExperiment::colData(mae[[1]]), mae[[1]])
```

---

remove_codrug_data	<i>Remove Codrug Data</i>
--------------------	---------------------------

---

**Description**

Remove Codrug Data

**Usage**

```
remove_codrug_data(
  data,
  prettify_identifiers = TRUE,
  codrug_identifiers = c("drug_name2", "concentration2")
)
```

**Arguments**

**data** data.table with input data  
**prettify\_identifiers** logical flag specifying if identifiers are expected to be prettified  
**codrug\_identifiers** character vector with identifiers for the codrug columns

**Value**

data.table without combination columns

**Examples**

```

dt <-
  data.table::data.table(
    "Drug Name" = letters[seq_len(3)],
    "Concentration" = seq_len(3),
    "Drug Name 2" = letters[4:6],
    "Concentration 2" = 4:6
  )
dt
remove_codrug_data(dt)

```

---

rename_bumpy	<i>Rename BumpyMatrix</i>
--------------	---------------------------

---

**Description**

Rename BumpyMatrix

**Usage**

```
rename_bumpy(bumpy, mapping_vector)
```

**Arguments**

**bumpy** a BumpyMatrix object  
**mapping\_vector** a named vector for mapping old and new values. The names of the character vector indicate the source names, and the corresponding values the destination names.

**Value**

a renamed BumpyMatrix object

**Examples**

```
mae <- get_synthetic_data("finalMAE_small.qs")
se <- mae[[1]]
assay <- SummarizedExperiment::assay(se)
rename_bumpy(assay, c("Concentration" = "conc"))
```

---

rename_DFrame	<i>Rename DFrame</i>
---------------	----------------------

---

**Description**

Rename DFrame

**Usage**

```
rename_DFrame(df, mapping_vector)
```

**Arguments**

`df` a DFrame object

`mapping_vector` a named vector for mapping old and new values. The names of the character vector indicate the source names, and the corresponding values the destination names.

**Value**

a renamed DFrame object

**Examples**

```
mae <- get_synthetic_data("finalMAE_small.qs")
rename_DFrame(SummarizedExperiment::rowData(mae[[1]]), c("Gnumber" = "Gnumber1"))
```

---

round_concentration	<i>Round concentration to ndigit significant digits</i>
---------------------	---

---

**Description**

Round concentration to ndigit significant digits

**Usage**

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



**Arguments**

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

**Value**

rounded x

**Examples**

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

---

set\_constant\_fit\_params

*Set fit parameters for a constant fit.*

---

**Description**

Replace values for flat fits: ec50 = 0, h = 0.0001 and xc50 = +/- Inf

**Usage**

```
set_constant_fit_params(out, mean_norm_value)
```

**Arguments**

out                    Named list of fit parameters.  
mean\_norm\_value        Numeric value that be used to set all parameters that can be calculated from the mean.

**Value**

Modified named list of fit parameters.

**Examples**

```
na <- list(x_0 = NA)  
set_constant_fit_params(na, mean_norm_value = 0.6)
```

---

SE_metadata	<i>Get and set metadata for parameters on a SummarizedExperiment object.</i>
-------------	--

---

## Description

Set metadata for the fitting parameters that define the Metrics assay in SummarizedExperiment object metadata.

## Usage

```
set_SE_fit_parameters(se, value)
set_SE_processing_metadata(se, value)
set_SE_keys(se, value)
set_SE_experiment_metadata(se, value)
set_SE_experiment_raw_data(se, value)
get_SE_fit_parameters(se)
get_SE_processing_metadata(se)
get_SE_experiment_raw_data(se)
get_SE_experiment_metadata(se)
get_SE_keys(se, key_type = NULL)
get_SE_identifiers(se, id_type = NULL, simplify = TRUE)
set_SE_identifiers(se, value)
```

## Arguments

se	a <a href="#">SummarizedExperiment</a> object for which to add fit parameter metadata.
value	named list of metadata for fit parameters.
key_type	string of a specific key type (i.e. 'nested_keys', etc.).
id_type	string of a specific id type (i.e. 'duration', 'cellline_name', etc.).
simplify	Boolean indicating whether output should be simplified.

**Details**

For `*et_SE_processing_metadata`, get/set metadata for the processing info that defines the `date_processed` and packages versions in `SummarizedExperiment` object metadata. For `*et_SE_fit_parameters`, get/set metadata for fit parameters used to construct the `Metrics` assay in a `SummarizedExperiment` object.

**Value**

se with added metadata.

**Examples**

```
mae <- get_synthetic_data("finalMAE_small.qs")
se <- mae[[1]]
get_SE_fit_parameters(se)
```

```
mae <- get_synthetic_data("finalMAE_small.qs")
se <- mae[[1]]
meta <- get_SE_processing_metadata(se)
```

```
mae <- get_synthetic_data("finalMAE_small.qs")
se <- mae[[1]]
get_SE_experiment_raw_data(se)
```

```
mae <- get_synthetic_data("finalMAE_small.qs")
se <- mae[[1]]
get_SE_experiment_metadata(se)
```

```
mae <- get_synthetic_data("finalMAE_small.qs")
se <- mae[[1]]
get_SE_identifiers(se)
```

---

shorten\_normalization\_type\_name  
*shorten normalization type*

---

**Description**

shorten normalization type

**Usage**

```
shorten_normalization_type_name(x)
```

**Arguments**

x string with normalization type

**Value**

shortened string representing the normalization type

**Examples**

```
shorten_normalization_type_name("GRvalue")
```

---

```
split_SE_components    split_SE_components
```

---

**Description**

Divide the columns of an input `data.table` into treatment metadata, condition metadata, experiment metadata, and assay data for further analysis. This will most commonly be used to identify the different components of a [SummarizedExperiment](#) object.

**Usage**

```
split_SE_components(df_, nested_keys = NULL, combine_on = 1L)
```

**Arguments**

<code>df_</code>	<code>data.table</code> with drug-response data
<code>nested_keys</code>	character vector of keys to exclude from the row or column metadata, and to instead nest within an element of the matrix. See details.
<code>combine_on</code>	integer value of 1 or 2, indicating whether unrecognized columns should be combined on row or column respectively. Defaults to 1.

**Details**

Named list containing the following elements:

**"treatment\_md"**: treatment metadata

**"condition\_md"**: condition metadata

**"data\_fields"**: all `data.table` column names corresponding to fields nested within a `BumpyMatrix` cell

**"experiment\_md"**: metadata that is constant for all entries of the `data.table`

**"identifiers\_md"**: key identifier mappings

The `nested_keys` provides the user the opportunity to specify that they would not like to use that metadata field as a differentiator of the treatments, and instead, incorporate it into a nested `DataFrame` in the `BumpyMatrix` matrix object.

In the event that if any of the `nested_keys` are constant throughout the whole `data.table`, they will still be included in the `DataFrame` of the `BumpyMatrix` and not in the `experiment_metadata`.

Columns within the `df_` will be identified through the following logic: First, the known data fields and any specified `nested_keys` are extracted. Following that, known cell and drug metadata fields are detected, and any remaining columns that represent constant metadata fields across all rows are extracted. Next, any cell line metadata will be heuristically extracted. Finally, all remaining columns will be combined on either the rows or columns as specified by `combine_on`.

### Value

named list containing different elements of a [SummarizedExperiment](#); see details.

### Examples

```
split_SE_components(data.table::data.table(clid = "CL1", Gnumber = "DrugA"))
```

---

standardize_mae	<i>Standardize MAE by switching from custom identifiers into gDR-default</i>
-----------------	--

---

### Description

Standardize MAE by switching from custom identifiers into gDR-default

### Usage

```
standardize_mae(mae, use_default = TRUE)
```

### Arguments

mae	a <code>MultiAssayExperiment</code> object with drug-response data generate by gDR pipeline
use_default	boolean indicating whether or not to use default identifiers for standardization

### Value

mae a `MultiAssayExperiment` with default gDR identifiers

### Examples

```
mae <- get_synthetic_data("finalMAE_small.qs")
S4Vectors::metadata(mae[[1]])$identifiers$drug <- "drug"
standardize_mae(mae)
```

---

standardize_se	<i>Standardize SE by switching from custom identifiers into gDR-default</i>
----------------	---

---

**Description**

Standardize SE by switching from custom identifiers into gDR-default

**Usage**

```
standardize_se(se, use_default = TRUE)
```

**Arguments**

se	a SummarizedExperiment object with drug-response data generate by gDR pipeline
use_default	boolean indicating whether or not to use default identifiers for standardization

**Value**

se a SummarizedExperiment with default gDR identifiers

**Examples**

```
mae <- get_synthetic_data("finalMAE_small.qs")
se <- mae[[1]]
S4Vectors::metadata(se)$identifiers$drug <- "drug"
standardize_se(se)
```

---

strip_first_and_last_char
---------------------------

*String first and last characters of a string.*

---

**Description**

String first and last characters of a string.

**Usage**

```
strip_first_and_last_char(jstring)
```

**Arguments**

jstring	String of any number of characters greater than 1.
---------	--

**Details**

This is most often used to remove the JSON brackets '{' and '}'.

**Value**

String with first and last characters stripped.

---

update\_env\_idfs\_from\_mae

*Update environment identifiers from MAE object identifiers*

---

**Description**

Update environment identifiers from MAE object identifiers

**Usage**

```
update_env_idfs_from_mae(mae_idfs)
```

**Arguments**

mae\_idfs            A list containing MAE identifiers

**Value**

NULL

**Examples**

```
update_env_idfs_from_mae(list(get_env_identifiers()))
```

---

update\_idfs\_synonyms    *Update gDR synonyms for the identifier*

---

**Description**

Update gDR synonyms for the identifier

**Usage**

```
update_idfs_synonyms(data, dict = get_idfs_synonyms())
```

**Arguments**

data                list of charvec with identifiers data  
dict                list with dictionary

**Value**

list

**Examples**

```
mdict <- list(duration = "time")
iv <- c("Time", "Duration", "time")
update_idfs_synonyms(iv, dict = mdict)
```

---

validate_dimnames	<i>Validate dimnames</i>
-------------------	--------------------------

---

**Description**

Assure that dimnames of two objects are the same

**Usage**

```
validate_dimnames(obj, obj2, skip_empty = TRUE)
```

**Arguments**

obj	first object with dimnames to compare
obj2	second object with dimnames to compare
skip_empty	a logical indicating whether to skip comparison if a given dimname is empty in the case of both objects

**Value**

NULL

---

validate_identifiers	<i>Check that specified identifier values exist in the data.</i>
----------------------	--

---

**Description**

Check that specified identifier values exist in the data and error otherwise.

**Usage**

```
validate_identifiers(
  df,
  identifiers = NULL,
  req_ids = NULL,
  exp_one_ids = NULL
)
```



**Arguments**

df	data.table with colnames.
identifiers	Named list of identifiers where the names are standardized identifier names. If not passed, defaults to <code>get_env_identifiers()</code> .
req_ids	Character vector of standardized identifier names required to pass identifier validation.
exp_one_ids	Character vector of standardized identifiers names where only one identifier value is expected. If not passed, defaults to <code>get_expect_one_identifiers()</code> .

**Details**

Note that this does NOT set the identifiers anywhere (i.e. environment or SummarizedExperiment object). If identifiers do not validate, will throw error as side effect.

**Value**

Named list of identifiers modified to pass validation against the input data. Errors with explanatory message if validation cannot pass with the given identifiers and data.

**Examples**

```
validate_identifiers(
  S4Vectors::DataFrame("Barcode" = NA, "Duration" = NA, "Template" = NA, "clid" = NA),
  req_ids = "barcode"
)
```

---

validate_json	<i>Validate JSON against a schema.</i>
---------------	--

---

**Description**

Validate JSON describing an object against a schema.

**Usage**

```
validate_json(json, schema_path)
```

**Arguments**

json	String of JSON in memory.
schema_path	String of the schema to validate against.

**Details**

This is most often used to validate JSON before passing it in as a document to an ElasticSearch index.

**Value**

Boolean of whether or not JSON successfully validated.

**Examples**

```
json <- '{}'
```

---

validate_MAE	<i>Validate MultiAssayExperiment object</i>
--------------	---

---

**Description**

Function validates correctness of SE included in MAE by checking multiple cases:

- detection of duplicated rowData/colData,
- incompatibility of rownames/colnames,
- occurrence of necessary assays,
- detection of mismatch of CLIDs inside colData and colnames (different order),
- correctness of metadata names.

**Usage**

```
validate_MAE(mae)
```

**Arguments**

mae                    MultiAssayExperiment object produced by the gDR pipeline

**Value**

NULL invisibly if the MultiAssayExperiment is valid. Throws an error if the MultiAssayExperiment is not valid.

**Author(s)**

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**Examples**

```
mae <- get_synthetic_data("finalMAE_small")  
validate_MAE(mae)
```

---

`validate_mae_with_schema`*Validate MAE against a schema.*

---

### Description

Validate MAE object against a schema. Currently only SEs are validated TODO: add mae.json schema and validate full MAE object

### Usage

```
validate_mae_with_schema(  
  mae,  
  schema_package = Sys.getenv("SCHEMA_PACKAGE", "gDRutils"),  
  schema_dir_path = Sys.getenv("SCHEMA_DIR_PATH", "schemas"),  
  schema = c(se = "se.json", mae = "mae.json")  
)
```

### Arguments

<code>mae</code>	MultiAssayExperiment object
<code>schema_package</code>	string name of the package with JSON schema files
<code>schema_dir_path</code>	path to the dir with JSON schema files
<code>schema</code>	named charvec with filenames of schemas to validate against.

### Value

Boolean of whether or not mae is valid

### Examples

```
mae <- get_synthetic_data("finalMAE_small")  
validate_mae_with_schema(mae)
```

---

`validate_SE`*Validate SummarizedExperiment object*

---

**Description**

Function validates correctness of SE by checking multiple cases:

- detection of duplicated rowData/colData,
- incompatibility of rownames/colnames,
- occurrence of necessary assays,
- detection of mismatch of CLIDs inside colData and colnames (different order),
- correctness of metadata names.

**Usage**

```
validate_SE(se, expect_single_agent = FALSE)
```

**Arguments**

`se` SummarizedExperiment object produced by the gDR pipeline  
`expect_single_agent` a logical indicating if the function should check whether the SummarizedExperiment is single-agent data

**Value**

NULL invisibly if the SummarizedExperiment is valid. Throws an error if the SummarizedExperiment is not valid.

**Examples**

```
mae <- get_synthetic_data("finalMAE_small")
se <- mae[[1]]
validate_SE(se)
```

---

```
validate_se_assay_name
```

*Check whether or not an assay exists in a SummarizedExperiment object.*

---

**Description**

Check for the presence of an assay in a SummarizedExperiment object.

**Usage**

```
validate_se_assay_name(se, name)
```

**Arguments**

se                    A [SummarizedExperiment](#) object.  
name                 String of name of the assay to validate.

**Value**

NULL invisibly if the assay name is valid. Throws an error if the assay is not valid.

**Examples**

```
mae <- get_synthetic_data("finalMAE_small")  
se <- mae[[1]]  
validate_se_assay_name(se, "RawTreated")
```

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