

# Package ‘gDRutils’

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**Type** Package

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

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**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.

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

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

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---

gDRutils-package	<i>gDRutils: A package with helper functions for processing drug response data</i>
------------------	------------------------------------------------------------------------------------

---

## 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.

## Value

package help page

## Note

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

## Author(s)

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

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- Marc Hafner ([ORCID](#))
- Pawel Piatkowski
- Dariusz Scigocki
- Janina Smola
- Sergiu Mocanu
- Allison Vuong

## See Also

Useful links:

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

---

```
.convert_mae_summary_to_json
```

*Create JSON document with MAE summary*

---

**Description**

Create JSON document with MAE summary, currently only experiment names

**Usage**

```
.convert_mae_summary_to_json(mae)
```

**Arguments**

mae                    MultiAssayExperiment object.

**Value**

String representation of a JSON document.

---

```
.convert_norm_specific_metrics
```

*This function change raw names of metric from long format table into more descriptive names in the wide format table. It works for metrics: colnames(get\_header("metrics\_names"))*

---

**Description**

This function change raw names of metric from long format table into more descriptive names in the wide format table. It works for metrics: colnames(get\_header("metrics\_names"))

**Usage**

```
.convert_norm_specific_metrics(x, normalization_type)
```

**Value**

object with more descriptive names

---

.prep\_cd\_conc\_cap\_dict

*Prepare dict with min and max concentration for codilution*

---

### Description

Prepare dict with min and max concentration for codilution

### Usage

```
.prep_cd_conc_cap_dict(  
  conc_assay_dt,  
  group_cols = as.character(get_env_identifiers(c("drug_name", "drug_name2",  
    "cellline_name"), simplify = FALSE))  
)
```

### Arguments

conc\_assay\_dt    assay data in data.table format with Concentration data  
group\_cols       charvec with grouping column names

### Value

data.table with max and min concentration for codilution

---

.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))
```

---

```
.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)
```

---

```
addClass
```

*add arbitrary S3 class to an object*

---

**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 `BumpyMatrix` 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	<i>assert choices</i>
----------------	-----------------------

---

**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	<i>Average biological replicates on the data table side.</i>
----------------------------------	--------------------------------------------------------------

---

**Description**

Average biological replicates on the data table side.

**Usage**

```
average_biological_replicates_dt(
  dt,
  var,
  prettified = FALSE,
  fixed = TRUE,
  geometric_average_fields = get_header("metric_average_fields")$geometric_mean,
  fit_type_average_fields = get_header("metric_average_fields")$fit_type,
  blacklisted_fields = get_header("metric_average_fields")$blacklisted,
  add_sd = FALSE
)
```

**Arguments**

dt	data.table with Metric data
var	String representing additional metadata of replicates
prettified	Flag indicating if the provided identifiers in the dt are prettified
fixed	Flag indicating whether to add a fix for -Inf in the geometric mean.
geometric_average_fields	Character vector of column names in dt to take the geometric average of.
fit_type_average_fields	Character vector of column names in dt that should be treated as a column with fit type data
blacklisted_fields	Character vector of column names in dt that should be skipped in averaging
add_sd	Flag indicating whether to add standard deviation and count columns.

**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")
```

---

calc\_sd

*Calculate Standard Deviation or Return Zero*

---

**Description**

This function calculates the standard deviation of a numeric vector. If the vector has a length of 1 and it is numeric, it returns 0.

**Usage**

```
calc_sd(x)
```

**Arguments**

x                    A numeric vector.

**Value**

The standard deviation of the vector if its length is greater than 1 or it is not numeric, otherwise 0.

**Examples**

```
calc_sd(c(1, 2, 3, 4, 5)) # Should return the standard deviation
calc_sd(c(1)) # Should return 0
calc_sd(numeric(0)) # Should return NA
calc_sd(c("a", "b", "c")) # Should return NA
```

---

capVals	<i>Cap metric values</i>
---------	--------------------------

---

**Description**

Convenience function to apply caps to outlying metric values.

**Usage**

```
capVals(x)
```

**Arguments**

x                      data.table containing growth metrics extracted from a SummarizedExperiment

**Details**

The following metrics are capped at the respective values:

- E max: 0 - 1.1
- GR max: -1 - 1.1
- RV AOC within set range: over -0.1
- GR AOC within set range: over of -0.1
- GR50: 1e-4 to 30
- IC50: 1e-4 to 30
- EC50: 1e-4 to 30 (change 0 to NA beforehand)

**Value**

A data table with capped values.

**See Also**

`convert_se_assay_to_dt`, [oob](#)

**Examples**

```
dt <- data.table::data.table(
  `E Max` = c(-0.1, 0, 0.5, 1.2),
  `GR Max` = c(-1.1, -1, 0.5, 1.2),
  `RV AOC within set range` = c(-0.2, -0.1, 0, 3),
  `GR AOC within set range` = c(-0.2, -0.1, 0, 3),
  `GR50` = c(0, 1e-7, 10, 34),
  `IC50` = c(0, 1e-7, 10, 34),
  `EC50` = c(0, 1e-7, 10, 34),
  check.names = FALSE
)
dt
dt1 <- capVals(dt)
dt1
```

---

cap\_assay\_infinities    *Cap infinity values (Inf, -Inf) in the assay data*

---

**Description**

Cap infinity values (Inf, -Inf) in the assay data

**Usage**

```
cap_assay_infinities(
  conc_assay_dt,
  assay_dt,
  experiment_name,
  col = "xc50",
  capping_fold = 5
)
```

**Arguments**

conc_assay_dt	assay data in data.table format with Concentration data
assay_dt	assay data in data.table format with infinity values to be capped
experiment_name	string with the name of the experiment
col	string with column name to be capped in assay_dt ("xc50" by default)
capping_fold	number for min and max concentration values final formulas are min / capping_fold and max * capping_fold

**Value**

data.table without -Inf / Inf values

**Examples**

```

# single-agent data
sdata <- get_synthetic_data("finalMAE_small")
smetrics_data <- convert_se_assay_to_dt(sdata[[get_supported_experiments("sa")]], "Metrics")
saveraged_data <- convert_se_assay_to_dt(sdata[[get_supported_experiments("sa")]], "Averaged")
smetrics_data_capped <- cap_assay_infinities(saveraged_data,
                                           smetrics_data,
                                           experiment_name = "single-agent")

# combination data
cdata <- get_synthetic_data("finalMAE_combo_matrix_small")
scaveraged_data <- convert_se_assay_to_dt(cdata[[get_supported_experiments("combo")]], "Averaged")
scmetrics_data <- convert_se_assay_to_dt(cdata[[get_supported_experiments("combo")]], "Metrics")
scmetrics_data_capped <- cap_assay_infinities(scaveraged_data,
                                              scmetrics_data,
                                              experiment_name = "combination")

```

---

cap\_xc50

*Cap XC50 value.*


---

**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**

cdata	data.table of colData.
identifiers	charvec with identifiers
req_cols	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

se	SummarizedExperiment object with dose-response data
c_assays	charvec of combo assays to be used
normalization_type	charvec of normalization_types expected in the data
prettify	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,  
  drop_masked = TRUE  
)
```

**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
drop_masked	Boolean indicating whether to drop masked values; TRUE by default.

**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,
  unify_metadata = FALSE,
  drop_masked = TRUE
)
```

## 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.
unify_metadata	Boolean indicating whether to unify DrugName and CellLineName in cases where DrugNames and CellLineNames are shared by more than one Gnumber and/or clid within the experiment.
drop_masked	Boolean indicating whether to drop masked values; TRUE by default.

## 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	<i>extend abbreviated normalization type</i>
--------------------------------	----------------------------------------------

---

**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

*Fit curves*


---

**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**

df_	data.table containing data to fit. See details.
series_identifiers	character vector of the column names in data.table whose combination represents a unique series for which to fit curves.
e_0	numeric value representing the x_0 value for the RV curve. Defaults to 1.
GR_0	numeric value representing the x_0 value for the GR curve. Defaults to 1.
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	numeric vector of length 2 indicating the lower and upper concentration ranges. Defaults to c(5e-3, 5). See details.
force_fit	boolean indicating whether or not to force a constant fit. Defaults to FALSE.
pcutoff	numeric of pvalue significance threshold above or equal to which to use a constant fit. Defaults to 0.05.

cap numeric value capping norm\_values to stay below  $(x_0 + \text{cap})$ . Defaults to 0.1.  
 normalization\_type character vector of types of curves to fit. Defaults to c("GR", "RV").

### 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

*Flatten a table*

---

### 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()
```

---

geometric_mean	<i>Geometric mean</i>
----------------	-----------------------

---

**Description**

Auxiliary function for calculating geometric mean with possibility to handle -Inf

**Usage**

```
geometric_mean(x, fixed = TRUE, maxlog10Concentration = 1)
```

**Arguments**

x	numeric vector
fixed	flag should be add fix for -Inf
maxlog10Concentration	numeric value needed to calculate minimal value

**Value**

numeric vector

**Examples**

```
geometric_mean(c(2, 8))
```

---

get_additional_variables	<i>Identify and return additional variables in list of dt</i>
--------------------------	---------------------------------------------------------------

---

**Description**

Identify and return additional variables in list of dt

**Usage**

```
get_additional_variables(dt_list, unique = FALSE, prettified = FALSE)
```



**Arguments**

dt_list	list of data.table or data.table containing additional variables
unique	logical flag indicating if all variables should be returned or only those containing more than one unique value
prettified	Flag indicating if the provided identifiers in the dt are prettified

**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\_dt\_duplicated\_rows

*Helper function to find duplicated rows in assay data*

---

**Description**

Helper function to find duplicated rows in assay data

**Usage**

```
get_assay_dt_duplicated_rows(dt, output = "index")
```

**Arguments**

dt	data.table
output	string with the output format to be returned

**Value**

integer vector or data.table with duplicated rows

**Examples**

```
sdata <- get_synthetic_data("finalMAE_small")  
smetrics_data <- convert_se_assay_to_dt(sdata[[1]], "Metrics")  
get_assay_dt_duplicated_rows(smetrics_data, output = "data")  
get_assay_dt_duplicated_rows(smetrics_data)
```

---

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_assay_req_uniq_cols	<i>get columns in the assay data required to have unique data</i>
-------------------------	-------------------------------------------------------------------

---

**Description**

get columns in the assay data required to have unique (non-duplicated) data

**Usage**

```
get_assay_req_uniq_cols(dt)
```

**Arguments**

dt	data.table with assay data
----	----------------------------

**Value**

charvec with columns required to have unique data

**Examples**

```
sdata <- get_synthetic_data("finalMAE_small")
smetrics_data <- convert_se_assay_to_dt(sdata[[1]], "Metrics")
get_assay_req_uniq_cols(smetrics_data)
```

---

`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**

<code>se</code>	SummarizedExperiment or NULL
<code>...</code>	Additional arguments to pass to <code>get_combo_assay_names</code> .

**Value**

charvec

**Author(s)**

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

**Examples**

```
get_combo_base_assay_names()
```

---

`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 <code>get_combo_assay_names</code> .

**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, output = "index")
```

**Arguments**

x	DataFrame or data.table
col_names	character vector, columns in which duplication are searched for
output	string with the output format to be returned - one of "index" (index of duplicates) or "data" (subset of input data with duplicates)

**Value**

integer vector or data.table with duplicated rows

**Examples**

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

---

get_env_assay_names	<i>get default assay names for the specified filters, i.e. set of assay types, assay groups and assay data types</i>
---------------------	----------------------------------------------------------------------------------------------------------------------

---

**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_env_var          safe wrapper of Sys.getenv()
```

---

**Description**

So far the helper is needed to handle env vars containing `:` for which the backslash is automatically added in some contexts and R could not get the original value for these env vars.

**Usage**

```
get_env_var(x, ...)
```

**Arguments**

`x` string with the name of the environmental variable  
`...` additional params for Sys.getenv

**Value**

sanitized value of the env variable

**Examples**

```
get_env_var("HOME")
```

---

```
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\_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**

<code>s</code>	charvec with setting entry/entries
<code>json_path</code>	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	<i>get_testdata_combo</i>
--------------------	---------------------------

---

**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_assay_dt_duplicated_rows	<i>check if assay data contains duplicated data</i>
------------------------------	-----------------------------------------------------

---

**Description**

An auxiliary function that checks for duplicates in the assay data

**Usage**

```
has_assay_dt_duplicated_rows(dt)
```

**Arguments**

dt                    data.table with assay data

**Value**

logical flag indicating if a dt contains duplicated rows or not

**Examples**

```
sdata <- get_synthetic_data("finalMAE_small")
smetrics_data <- convert_se_assay_to_dt(sdata[[1]], "Metrics")
has_assay_dt_duplicated_rows(smetrics_data)
```

has\_dt\_duplicated\_rows

*check if data.table contains duplicated data*

---

### Description

An auxiliary function that checks for duplicates in the data.table (or its subset)

### Usage

```
has_dt_duplicated_rows(dt, col_names = NULL)
```

### Arguments

dt	data.table
col_names	charvec with columns to be used for subsetting

### Value

logical flag indicating if a dt contains duplicated rows or not

### Examples

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

---

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

*Get or reset headers for one or all header field(s) respectively*

---

**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`*Get, set, or reset identifiers for one or all identifier field(s)*

---

### 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

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

### 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)
```

---

<i>is_any_exp_empty</i>	<i>is_any_exp_empty</i>
-------------------------	-------------------------

---

**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)
```

---

is_exp_empty	<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.
pcutoff	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 + 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: <https://screener.genedata.com/documentation/display/DOC21/Business-Rules-for-Dose-Response-Curve-Fitting,-Model-Selection,-and-Fit-Validity.html> #nolint

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	<i>Lapply through all the experiments in MultiAssayExperiment object</i>
----------	--------------------------------------------------------------------------

---

**Description**

Lapply through all the experiments in MultiAssayExperiment object

**Usage**

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

**Arguments**

mae	MultiAssayExperiment object
FUN	function that should be applied on each experiment of MultiAssayExperiment object
unify	logical indicating if the output should be a unlisted object of unique values across all the experiments
...	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")
MAEply(mae, SummarizedExperiment::assayNames)
```

---

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.

**Examples**

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

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

map_conc_to_standardized_conc(concl, conc2)
```

---

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**

efficacy	Numeric vector representing efficacies to predict concentrations 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

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

---

```
predict_efficity_from_conc
```

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

---

**Description**

Predict efficacy values given fit parameters and a concentration.

**Usage**

```
predict_efficity_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_efficity`.

**Value**

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

**See Also**

`predict_conc_from_efficity`

**Examples**

```
predict_efficity_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)
```

---

refine_coldata	<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**

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

**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      *Remove Codrug Data*

---

**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)
```



---

remove_drug_batch	<i>Remove batch substring from drug id</i>
-------------------	--------------------------------------------

---

### Description

Gnumber, i.e. "G12345678" is currently the default format of drug\_id. It's also used as a drug name in some cases.

### Usage

```
remove_drug_batch(
  drug_vec,
  drug_p = "^G[0-9]{8}",
  sep_p = "[^0-9|^_]",
  batch_p = ".+"
)
```

### Arguments

drug_vec	character vector with drug id(s)
drug_p	string with regex pattern for drug id. Set to Gnumber format by default: "G[0-9]{8}".
sep_p	string with regex pattern for separator. Set to any character except for digit and space
batch_p	string with regex pattern for batch substring. By default set to any character(s): "+."

### Details

By default, Gnumber(s) followed by any character (except for underscore and any digit) and any batch substring are cleaned:

- G00060245.18 => G00060245
- G00060245.1-8 => G00060245
- G02948263.1-1.DMA => G02948263
- Gnumber followed by the codrug
  - G03252046.1-2;G00376771 => G03252046
- Gnumber followed by the two codrugs
  - G03256376.1-2;G00376771.1-19;G02557755 => G03256376
- Gnumber followed by the drug name
  - G00018838, Cisplatin => G00018838

By default, Gnumber(s) followed by the "\_" or digit (regardless the batch substring) are not cleaned:

- Gnumber with suffix added to prevent duplicated ids

- G00060245\_(G00060245.1-8)
- too long Gnumber
- G123456789.1-12

**Value**

charvec with Gnumber(s)

**Examples**

```
remove_drug_batch("G00060245.18")
remove_drug_batch("G00060245.1-8")
remove_drug_batch("G00060245.1-1.DMA")

remove_drug_batch("G03252046.1-2;G00376771")
remove_drug_batch("G00018838, Cisplatin")
remove_drug_batch("G03256376.1-2;G00376771.1-19;G02557755")
remove_drug_batch("G00060245_(G00060245.1-8)")
remove_drug_batch(c("G00060245.18", "G00060245.1-8", "G00060245.1-1.DMA"))

remove_drug_batch("DRUG_01.123", drug_p = "DRUG_[0-9]+")
remove_drug_batch("G00001234:22-1", sep_p = ":")
remove_drug_batch("G00001234.28", batch_p = "[0-9]+")
```

---

rename\_bumpy

*Rename BumpyMatrix*

---

**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)
```

---

set\_unique\_cl\_names     *Set Unique Parental Identifiers*

---

### Description

This function sets the CellLineName field in colData to be unique by appending the clid in parentheses for duplicates.

### Usage

```
set_unique_cl_names(se)
```

### Arguments

se                    A SummarizedExperiment object.

### Value

A SummarizedExperiment object with unique CellLineName in colData.

### Examples

```
se <- SummarizedExperiment::SummarizedExperiment(  
  assays = list(counts = matrix(1:4, ncol = 2)),  
  colData = S4Vectors::DataFrame(CellLineName = c("ID1", "ID1"), clid = c("C1", "C2"))  
)  
se <- set_unique_cl_names(se)
```

---

set\_unique\_cl\_names\_dt

*Set unique primary cell line identifiers in the table*

---

### Description

This function sets the primary cell line field in data.frame-like object to be unique by appending the secondary cell line field in parentheses for duplicates.

### Usage

```
set_unique_cl_names_dt(  
  dt,  
  primary_name = get_env_identifiers("cellline_name"),  
  secondary_name = get_env_identifiers("cellline"),  
  sep = " "  
)
```

**Arguments**

dt                    data.table, data.frame or DFrame with the data  
 primary\_name        string with the name of the primary cell line field  
 secondary\_name      string with the name of the secondary cell line field  
 sep                   string with separator added before suffix

**Value**

fixed input table with unique primary cell line field in dt

**Examples**

```
col_data <- S4Vectors::DataFrame(CellLineName = c("ID1", "ID1"), clid = c("C1", "C2"))
col_data <- set_unique_cl_names_dt(col_data)
```

---

set\_unique\_drug\_names    *Set Unique Drug Names*

---

**Description**

This function sets the DrugName, DrugName\_2, and DrugName\_3 fields in rowData to be unique by appending the corresponding Gnumber, Gnumber\_2, and Gnumber\_3 in parentheses for duplicates.

**Usage**

```
set_unique_drug_names(se)
```

**Arguments**

se                    A SummarizedExperiment object.

**Value**

A SummarizedExperiment object with unique DrugName fields in rowData.

**Examples**

```
se <- SummarizedExperiment::SummarizedExperiment(
  assays = list(counts = matrix(1:9, ncol = 3)),
  rowData = S4Vectors::DataFrame(DrugName = c("DrugA", "DrugA", "DrugB"),
  Gnumber = c("G1", "G2", "G5"),
  DrugName_2 = c("DrugC", "DrugC", "DrugD"),
  Gnumber_2 = c("G3", "G4", "G5")
))
se <- set_unique_drug_names(se)
```

---

 set\_unique\_drug\_names\_dt

*Set unique primary drug identifiers in the table*


---

## Description

This function sets the primary drug field(s) in data.frame-like object to be unique by appending the secondary drug field(s) in parentheses for duplicates. By default DrugName, DrugName\_2, and DrugName\_3 are primary drug fields, while Gnumber, Gnumber\_2, and Gnumber\_3 are their respective secondary drug fields.

## Usage

```
set_unique_drug_names_dt(
  dt,
  primary_names = unlist(get_env_identifiers()[c("drug_name", "drug_name2",
    "drug_name3")]),
  secondary_names = unlist(get_env_identifiers()[c("drug", "drug2", "drug3")]),
  sep = " "
)
```

## Arguments

dt	data.table, data.frame or DFrame with the data
primary_names	charvec with the names of the primary drug field(s)
secondary_names	charvec with the name of the secondary drug field(s)
sep	string with separator added before suffix

## Value

fixed input table with unique primary drug field in dt

## Examples

```
row_data <- S4Vectors::DataFrame(
  DrugName = c("DrugA", "DrugA", "DrugB"),
  Gnumber = c("G1", "G2", "G5"),
  DrugName_2 = c("DrugC", "DrugC", "DrugD"),
  Gnumber_2 = c("G3", "G4", "G5")
)
row_data <- set_unique_drug_names_dt(row_data)
```

---

`set_unique_identifiers`*Set Unique Identifiers in MultiAssayExperiment*

---

## Description

This function sets the CellLineName in colData and DrugName fields in rowData to be unique for each SummarizedExperiment in a MultiAssayExperiment.

## Usage

```
set_unique_identifiers(mae)
```

## Arguments

`mae` A MultiAssayExperiment object.

## Value

A MultiAssayExperiment object with unique identifiers.

## Examples

```
se1 <- SummarizedExperiment::SummarizedExperiment(  
  assays = list(counts = matrix(1:4, ncol = 2)),  
  colData = S4Vectors::DataFrame(parental_identifier = c("ID1", "ID1"), clid = c("C1", "C2")),  
  rowData = S4Vectors::DataFrame(DrugName = c("DrugA", "DrugA"), Gnumber = c("G1", "G2"))  
)  
rownames(SummarizedExperiment::colData(se1)) <- c("c11", "c12")  
rownames(SummarizedExperiment::rowData(se1)) <- c("g1", "g")  
se2 <- SummarizedExperiment::SummarizedExperiment(  
  assays = list(counts = matrix(5:8, ncol = 2)),  
  colData = S4Vectors::DataFrame(parental_identifier = c("ID2", "ID2"), clid = c("C3", "C4")),  
  rowData = S4Vectors::DataFrame(DrugName = c("DrugB", "DrugB"), Gnumber = c("G3", "G4"))  
)  
rownames(SummarizedExperiment::colData(se2)) <- c("c13", "c14")  
rownames(SummarizedExperiment::rowData(se2)) <- c("g3", "g4")  
mae <- MultiAssayExperiment::MultiAssayExperiment(experiments = list(se1 = se1, se2 = se2))  
mae <- set_unique_identifiers(mae)
```



---

set\_unique\_names\_dt     *Set unique primary identifiers in the data.frame-like objects*

---

### Description

This function sets the primary field in the data.frame-like objects to be unique by appending the secondary field in parentheses for duplicates.

### Usage

```
set_unique_names_dt(dt, primary_name, secondary_name, sep = " ")
```

### Arguments

dt	data.table, data.frame or DFrame with data
primary_name	string with the name of the primary field
secondary_name	string with the name of the secondary field
sep	string with separator added before suffix

### Value

fixed input table with unique primary field in the table

### Examples

```
col_data <- S4Vectors::DataFrame(CellLineName = c("ID1", "ID1"), clid = c("C1", "C2"))
col_data <- set_unique_names_dt(col_data, primary_name = "CellLineName", secondary_name = "clid")
```

---

SE\_metadata     *Get and set metadata for parameters on a SummarizedExperiment object.*

---

### 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>	data.table 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 MultiAssayExperiment 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 <- "druug"
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.

---

```
throw_msg_if_duplicates
```

*throw message if assay data.table contains duplicated rows*

---

### Description

An auxiliary function that checks for duplicated rows in assay data.table, In case of duplicates it throws a message. The message function is by default stop() The message function can be customized with msg\_f parameter

### Usage

```
throw_msg_if_duplicates(  
  dt,  
  assay_name = "unknown",  
  msg_f = stop,  
  preview_max_numb = 4  
)
```

### Arguments

dt	data.table with assay data
assay_name	string with the name of the assay
msg_f	function to be used to throw the message
preview_max_numb	number of rows to preview if duplicates found

### Examples

```
sdata <- get_synthetic_data("finalMAE_small")  
smetrics_data <- convert_se_assay_to_dt(sdata[[1]], "Metrics")  
throw_msg_if_duplicates(smetrics_data, assay_name = "Metrics", msg_f = futile.logger::flog.info)
```

---

```
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)

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

## 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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