

# Package ‘gDRutils’

December 17, 2025

**Type** Package

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

**Version** 1.9.4

**Date** 2025-12-02

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

**License** Artistic-2.0

**LazyLoad** yes

**Depends** R (>= 4.2)

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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)

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## 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))
```

---

```
.snap_conc_to_model
```

*Snap a concentration to the nearest available model concentration*


---

**Description**

Finds the value in a vector of available concentrations that is closest (on a log scale) to a user-specified concentration. This is an internal helper function.

**Usage**

```
.snap_conc_to_model(user_conc, available_concs)
```

**Arguments**

`user_conc`            A single numeric value for the desired concentration.  
`available_concs`       A numeric vector of concentrations for which a model exists.

**Value**

A single numeric value from 'available\_concs'.

---

```
.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 | <i>Apply a function to every element of a bumpy matrix.</i> |
|----------------------|-------------------------------------------------------------|

---

**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.<br>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 checkmate::test_choice |

**Value**

NULL

**Examples**

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

---

```
average_biological_replicates_dt
```

*Average biological replicates on the data table side.*

---

**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(seq_len(10), 1),
  b = c(rep("drugA", 10), rep("drugB", 1)))
average_biological_replicates_dt(dt, var = "a")
```

---

|                 |                                                                                                                                                                                            |
|-----------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| average_pvalues | <i>Average p-values using Fisher's method Combines a vector of p-values into a single representative p-value. It implements Fisher's method, where the test statistic is calculated as</i> |
|-----------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|

$$X_{2k}^2 = -2 \sum_{i=1}^k \ln(p_i)$$

. This statistic follows a chi-squared distribution with  $2k$  degrees of freedom (where  $k$  is the number of p-values), from which the combined p-value is derived.

---

**Description**

Average p-values using Fisher's method Combines a vector of p-values into a single representative p-value. It implements Fisher's method, where the test statistic is calculated as

$$X_{2k}^2 = -2 \sum_{i=1}^k \ln(p_i)$$

. This statistic follows a chi-squared distribution with  $2k$  degrees of freedom (where  $k$  is the number of p-values), from which the combined p-value is derived.

**Usage**

```
average_pvalues(p_values)
```

**Arguments**

|          |                                                                                                                                      |
|----------|--------------------------------------------------------------------------------------------------------------------------------------|
| p_values | A numeric vector of p-values. Values are expected to be between 0 and 1. The function assumes at least one non-NA value is provided. |
|----------|--------------------------------------------------------------------------------------------------------------------------------------|

**Value**

A single, combined p-value as a numeric value.

---

`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`*Cap metric values*

---

**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

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

|                       |                                                                                                                                                                                                                                                                                                                            |
|-----------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 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                                                                                                                                                                                                                   |
| additional_group_cols | character vector of column names used to identify unique observations <ul style="list-style-type: none"><li>• for single-agent experiment additional to the combination of DrugName and CellLineName</li><li>• for combination experiment additional to the combination of DrugName, DrugName_2 and CellLineName</li></ul> |

## data.table without -Inf / Inf values

[illegible]



---

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

---

## Description

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

## Usage

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

## Arguments

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

## Details

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

## Value

Capped IC50/GR50 value.

## Examples

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

---

`convert_colData_to_json`*Convert colData to JSON*

---

### Description

Convert colData to JSON format for elasticsearch indexing.

### Usage

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

### Arguments

|             |                          |
|-------------|--------------------------|
| 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**

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

**Value**

list of data.table(s) with combo data

**Author(s)**

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

**Examples**

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

---

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

---

**Description**

get combo assay names based on the field name

**Usage**

```
convert_combo_field_to_assay(field)
```

**Arguments**

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

**Value**

charvec

**Examples**

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

---

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

---

**Description**

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

**Usage**

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

**Arguments**

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

**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**

|                          |                          |
|--------------------------|--------------------------|
| <code>rdata</code>       | data.table of rowData.   |
| <code>identifiers</code> | charvec with identifiers |
| <code>req_cols</code>    | 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,
  cap_values = FALSE
)
```

## 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.                                                     |
| cap_values   | Logical indicating whether to apply capping (via capVals) for "Metrics" output. Default is FALSE. |

## 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 + cap\_values if cap\_values = TRUE)

#### 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 the 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_custom_dt(se, "Metrics", cap_values = TRUE)
```

---

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,
  merge_additional_variables = FALSE
)
```

**Arguments**

|                            |                                                                                                                                                                                                                                                                                                                                                                        |
|----------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| se                         | A <a href="#">SummarizedExperiment</a> object holding raw and/or processed dose-response data in its assays.                                                                                                                                                                                                                                                           |
| assay_name                 | String of name of the assay to transform within the se.                                                                                                                                                                                                                                                                                                                |
| include_metadata           | Boolean indicating whether or not to include <code>rowData(se)</code> and <code>colData(se)</code> in the returned <code>data.table</code> . Defaults to TRUE.                                                                                                                                                                                                         |
| retain_nested_rownames     | Boolean indicating whether or not to retain the rownames nested within a <code>BumpyMatrix</code> assay. Defaults to FALSE. If the <code>assay_name</code> is not of the <code>BumpyMatrix</code> class, this argument's value is ignored. If TRUE, the resulting column in the <code>data.table</code> will be named as " <code>&lt;assay_name&gt;_rownames</code> ". |
| wide_structure             | Boolean indicating whether or not to transform <code>data.table</code> into wide format. <code>wide_structure = TRUE</code> requires <code>retain_nested_rownames = TRUE</code> .                                                                                                                                                                                      |
| unify_metadata             | Boolean indicating whether to unify <code>DrugName</code> and <code>CellLineName</code> in cases where <code>DrugNames</code> and <code>CellLineNames</code> are shared by more than one <code>Gnumber</code> and/or <code>clid</code> within the experiment.                                                                                                          |
| drop_masked                | Boolean indicating whether to drop masked values; TRUE by default.                                                                                                                                                                                                                                                                                                     |
| merge_additional_variables | Boolean indicating whether to merge additional variables identified by <code>get_additional_variables</code> into the <code>DrugName</code> column. Defaults to FALSE.                                                                                                                                                                                                 |

**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 | <i>Convert a SummarizedExperiment object to a JSON document.</i> |
|--------------------|------------------------------------------------------------------|

---

**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")
```

---

|                             |                       |
|-----------------------------|-----------------------|
| <code>df_to_bm_assay</code> | <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"))
```

---

|                                             |                                              |
|---------------------------------------------|----------------------------------------------|
| <code>extend_normalization_type_name</code> | <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 | <i>Fit curves</i> |
|------------|-------------------|

---

**Description**

Fit GR and RV curves from a data.table.

**Usage**

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

**Arguments**

|                    |                                                                                                                          |
|--------------------|--------------------------------------------------------------------------------------------------------------------------|
| 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 + 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 | <i>Flatten a table</i> |
|---------|------------------------|

---

**Description**

Flatten a stacked table into a wide format.

**Usage**

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

**Arguments**

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



**Details**

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

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

**Value**

table of flattened data as defined by wide\_cols.

**See Also**

convert\_se\_assay\_to\_dt

**Examples**

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

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

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

---

|                    |                           |
|--------------------|---------------------------|
| gen_synthetic_data | <i>gen_synthetic_data</i> |
|--------------------|---------------------------|

---

**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**

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

**Value**

charvec

**Author(s)**

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

**Examples**

```
get_combo_base_assay_names()
```

---

get\_combo\_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

|                  |                                                                      |
|------------------|----------------------------------------------------------------------|
| <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_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 | <i>safe wrapper of Sys.getenv()</i> |
|-------------|-------------------------------------|

---

**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 | <i>Get identifiers that expect only one value for each identifier.</i> |
|----------------------------|------------------------------------------------------------------------|

---

**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_gDR_session_info` *get gDR package and their version installed in the environment*

---

**Description**

get gDR package and their version installed in the environment

**Usage**

```
get_gDR_session_info(pattern = "^gDR")
```

**Arguments**

`pattern` string with the pattern to grep R packages from the list of installed packages

**Value**

data.table with gDR packages and their versions

**Examples**

```
get_gDR_session_info()
```

---

|                    |                                         |
|--------------------|-----------------------------------------|
| get_identifiers_dt | <i>Get descriptions for identifiers</i> |
|--------------------|-----------------------------------------|

---

**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
```

*Get isobologram column names*

---

**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", "settings.json")  
)
```

### Arguments

|           |                                       |
|-----------|---------------------------------------|
| s         | charvec with setting entry/entries    |
| json_path | string with the path to the JSON file |

### Value

value/values for entry/entries from JSON file



**Examples**

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

---

|                                        |  |
|----------------------------------------|--|
| <code>get_supported_experiments</code> |  |
| <i>get_supported_experiments</i>       |  |

---

**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 | <i>Get synthetic data from gDRtestData package</i> |
|--------------------|----------------------------------------------------|

---

**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 | <i>get_testdata</i> |
|--------------|---------------------|

---

**Description**

Function to obtain data from gDRtestData and prepare for unit tests

**Usage**

```
get_testdata()
```

**Value**

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

**Examples**

```
get_testdata()
```

---

```
get_testdata_codilution  
    get_testdata_codilution
```

---

**Description**

Function to obtain data from gDRtestData and prepare for unit tests

**Usage**

```
get_testdata_codilution()
```

**Value**

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

**Examples**

```
get_testdata_codilution()
```

---

```
get_testdata_combo    get_testdata_combo
```

---

**Description**

Function to obtain data from gDRtestData and prepare for unit tests

**Usage**

```
get_testdata_combo()
```

**Value**

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

**Examples**

```
get_testdata_combo()
```

---

has\_assay\_dt\_duplicated\_rows  
*check if assay data contains duplicated data*

---

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

---

**Description**

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

**Usage**

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

**Arguments**

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

**Details**

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

**Value**

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

**Examples**

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

---

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

---

**Description**

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

**Usage**

```
get_env_identifiers(k = NULL, simplify = TRUE)

get_prettified_identifiers(k = NULL, simplify = TRUE)

set_env_identifier(k, v)

reset_env_identifiers()
```

**Arguments**

|                       |                                                                                   |
|-----------------------|-----------------------------------------------------------------------------------|
| <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)
```

---

`is_any_exp_empty`                  *is\_any\_exp\_empty*

---

**Description**

check if any experiment is empty

**Usage**

```
is_any_exp_empty(mae)
```

**Arguments**

mae                      MultiAssayExperiment object

**Value**

logical

**Author(s)**

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

**Examples**

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

---

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

---

**Description**

Checks if se is combo dataset.

**Usage**

```
is_combo_data(se)
```

**Arguments**

se SummarizedExperiment

**Value**

logical

**Examples**

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

---

|              |              |
|--------------|--------------|
| is_exp_empty | is_exp_empty |
|--------------|--------------|

---

**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)
```

---

|              |              |
|--------------|--------------|
| is_mae_empty | is_mae_empty |
|--------------|--------------|

---

**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. |

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

---

*Conditional lapply or bplapply with optional batch processing.*


---

## Description

Conditional lapply or bplapply with optional batch processing.

## Usage

```
loop(
  x,
  FUN,
  parallelize = TRUE,
  use_batch = as.logical(Sys.getenv("GDR_USE_BATCH", "FALSE")),
  temp_dir = Sys.getenv("GDR_TEMP_DIR", tempdir()),
  batch_size = as.numeric(Sys.getenv("GDR_BATCH_SIZE", 100)),
  ...
)
```

## Arguments

|             |                                                                                                                                       |
|-------------|---------------------------------------------------------------------------------------------------------------------------------------|
| x           | Vector (atomic or list) or an expression object. Other objects (including classed objects) will be coerced by <a href="#">as.list</a> |
| FUN         | A user-defined function to apply to each element of x.                                                                                |
| parallelize | Logical indicating whether or not to parallelize the computation. Defaults to TRUE.                                                   |
| use_batch   | Logical indicating whether to use batch processing to save intermediate results. Defaults to FALSE.                                   |
| temp_dir    | Character string specifying the directory where batch results are saved. Defaults to tempdir().                                       |
| batch_size  | Integer specifying the number of elements to process in each batch during batch mode. Defaults to 100.                                |
| ...         | Optional arguments passed to <a href="#">bplapply</a> if parallelize == TRUE, else to <a href="#">lapply</a> .                        |

## Details

The function operates in two modes:

1. Regular mode: Directly applies FUN to the elements using lapply or bplapply.
2. Batch mode: Saves results in batches to disk, allowing computation to resume from the last saved step. Batch mode is activated by setting use\_batch to TRUE.

## Value

List containing output of FUN applied to every element in x. When batch processing is enabled, results are saved incrementally and merged at the end of processing.

## Examples

```
# Regular processing
loop(list(1, 2, 3), function(x) x^2, parallelize = FALSE, use_batch = FALSE)

# Batch processing
loop(1:10, function(x) x^2, parallelize = TRUE, use_batch = TRUE)
```

---

MAEapply

*Apply through all the experiments in MultiAssayExperiment object*

---

## Description

Apply 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
conc1 <- c(0, 10 ^ (seq(-3, 1, ratio)))

shorter_range <- conc1[-1]
noise <- runif(length(shorter_range), 1e-12, 1e-11)
conc2 <- shorter_range + noise

map_conc_to_standardized_conc(conc1, conc2)
```



---

|          |                 |
|----------|-----------------|
| mcolData | <i>mcolData</i> |
|----------|-----------------|

---

**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\_MAE

---

Merge multiple MultiAssayExperiment objects

---

**Description**

Merge multiple MultiAssayExperiment objects

**Usage**

```
merge_MAE(
  MAElist,
  additional_col_name = "data_source",
  discard_keys = c("normalization_type", "fit_source", "record_id", "isDay0", "swap_sa",
    "control_type", "iso_level", "conc_1", "conc_2")
)
```

**Arguments**

|                     |                                                                                                                                                               |
|---------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------|
| MAElist             | Named list of MultiAssayExperiment objects.                                                                                                                   |
| 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 strings that will be discarded during creating BumpyMatrix object.                                                                        |

**Value**

Merged MultiAssayExperiment object.

**Examples**

```
mae1 <- get_synthetic_data("finalMAE_combo_2dose_nonoise")
mae2 <- get_synthetic_data("finalMAE_combo_2dose_nonoise")
merge_MAE(list(mae1 = mae1, mae2 = mae2))
```

---

|                |                       |
|----------------|-----------------------|
| 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", "isDay0", "swap_sa",  
    "control_type", "iso_level", "conc_1", "conc_2")  
)
```

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

---

predict\_efficacy\_from\_conc

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

---

**Description**

Predict efficacy values given fit parameters and a concentration.

**Usage**

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

**Arguments**

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

**Details**

The inverse of this function is predict\_conc\_from\_efficacy.

**Value**

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

**See Also**

predict\_conc\_from\_efficacy

**Examples**

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

---

predict\_smooth\_from\_combo

*Predict a smoothed response for a drug combination*

---

**Description**

Predicts a 'smooth' value for a single pair of drug concentrations by snapping to the nearest available models from a metrics table and averaging their predictions. This is the combination equivalent of 'predict\_efficacy\_from\_conc'.

**Usage**

```
predict_smooth_from_combo(conc_1, conc_2, metrics_merged)
```

**Arguments**

|                |                                                                                                                                                         |
|----------------|---------------------------------------------------------------------------------------------------------------------------------------------------------|
| conc_1         | A single numeric value for the desired concentration of the first drug.                                                                                 |
| conc_2         | A single numeric value for the desired concentration of the second drug.                                                                                |
| metrics_merged | A data.table containing all pre-calculated curve fit parameters. Expects columns: 'dilution_drug', 'cotrt_value', 'ratio', 'ec50', 'h', 'x_inf', 'x_0'. |



**Value**

A single numeric value for the predicted 'smooth' response.

**Examples**

```
mae <- gDRutils::get_synthetic_data("combo_matrix")
se <- mae[[gDRutils::get_supported_experiments("combo")]]
dt_metrics <- gDRutils::convert_se_assay_to_dt(se[1, 1], "Metrics")[normalization_type == "RV"]
predict_smooth_from_combo(conc_1 = 1.2, conc_2 = 9.8, metrics_merged = dt_metrics)
```

---

```
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)
```

---

process\_batch

*Process and save a batch of results.*


---

**Description**

Process and save a batch of results.

**Usage**

```
process_batch(
  batch,
  start_index,
  fun_name,
  unique_id,
  total_iterations,
  temp_dir,
  FUN,
  ...
)
```

**Arguments**

|                  |                                                                                        |
|------------------|----------------------------------------------------------------------------------------|
| batch            | A subset of the vector or list x to be processed.                                      |
| start_index      | Integer indicating the starting index of the batch in the original vector x.           |
| fun_name         | Character string representing the name of the function FUN for use in file naming.     |
| unique_id        | String with unique identifier for the current task and user to ensure file uniqueness. |
| total_iterations | Integer indicating the total number of iterations in the original vector x.            |
| temp_dir         | Character string specifying the directory where batch results are saved.               |
| FUN              | A user-defined function to apply to each element of the batch.                         |
| ...              | Optional arguments passed to FUN.                                                      |

**Details**

The function applies FUN to each element in batch, saves the results to a file named according to the format <fun\_name>\_<unique\_id>\_<start\_index>\_of\_<total\_iterations>\_batch.qs, and clears memory using gc() after saving.

**Value**

This function does not return a value. It saves the processed batch results to disk as a .qs file.

**Examples**

```
process_batch(list(1, 2, 3), 100, "my_function", "unique_task_id_user", 1000, tempdir(), function(x) x^2)
```

---

|                |                                                                                                                                   |
|----------------|-----------------------------------------------------------------------------------------------------------------------------------|
| 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 meta-data 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 | <i>Remove Codrug Data</i> |
|--------------------|---------------------------|

---

**Description**

Remove Codrug Data

**Usage**

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

**Arguments**

data                      data.table with input data

prettify\_identifiers                      logical flag specifying if identifiers are expected to be prettified

codrug\_identifiers                      character vector with identifiers for the codrug columns

**Value**

data.table without combination columns

**Examples**

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

---

|                   |                                            |
|-------------------|--------------------------------------------|
| 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 | <i>Set Unique Parental Identifiers</i> |
|---------------------|----------------------------------------|

---

**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 | <i>Set unique primary cell line identifiers in the table</i> |
|------------------------|--------------------------------------------------------------|

---

**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 | <i>Set unique primary identifiers in the data.frame-like objects</i> |
|---------------------|----------------------------------------------------------------------|

---

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

---

**Description**

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

**Usage**

```
set_SE_fit_parameters(se, value)

set_SE_processing_metadata(se, value)

set_SE_keys(se, value)

set_SE_experiment_metadata(se, value, append = TRUE)

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.                                             |
| append   | Boolean indicating whether to append the new metadata value to the existing entry.     |
| 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\_big\_table\_for\_xlsx

*Split big table*


---

### Description

Helper function for saving big tables in an Excel file. Excel has a sheet size limit, if the table is too large it will not be possible to save such a file. This function allows you to split the table into smaller parts so that saving can be possible

### Usage

```
split_big_table_for_xlsx(dt_list, max_row = 1e+06, max_col = 16000)
```

### Arguments

|         |                                                                                                                                                                                                       |
|---------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| dt_list | list of data.tables. Each data.table will be checked and split if meet the criteria                                                                                                                   |
| max_row | integer defining the maximum number of rows in one sheet, the rows will be divided into portions of this size. Default value, 1 000 000, is based on excel limit - 1 048 576 with extra safety margin |
| max_col | integer defining the maximum number of columns in one sheet, the columns will be divided into portions of this size. Default value, 16 000, is based on excel limit - 16 384 with extra safety margin |

### Value

list of data.tables

### Examples

```
too_large_dt <- list(data.table::data.table(matrix(seq_len(300)), nrow = 10))
split_big_table_for_xlsx(too_large_dt, max_row = 250)
```

---

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 <- "drug"
standardize_mae(mae)
```

---

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

---

**Description**

Standardize SE by switching from custom identifiers into gDR-default

**Usage**

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

**Arguments**

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

**Value**

se a SummarizedExperiment with default gDR identifiers

### Examples

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

---

strip\_first\_and\_last\_char

*String first and last characters of a string.*

---

### Description

String first and last characters of a string.

### Usage

```
strip_first_and_last_char(jstring)
```

### Arguments

jstring               String of any number of characters greater than 1.

### Details

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

### Value

String with first and last characters stripped.

---

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_drug_name | <i>Update drug name with additional variables</i> |
|------------------|---------------------------------------------------|

---

**Description**

Concatenates the values of specified additional variables to the existing drug identifier columns in a data.table, using the variables defined in `get_env_identifiers`.

**Usage**

```
update_drug_name(dt, additional_vars)
```

**Arguments**

|                 |                                                                                                                                         |
|-----------------|-----------------------------------------------------------------------------------------------------------------------------------------|
| dt              | A data.table containing drug-response information, including drug identifier columns (e.g., DrugName, Gnumber) and the additional_vars. |
| additional_vars | Character vector of column names (variables) to merge into the drug identifier columns.                                                 |

**Value**

A copy of the input data.table dt with the relevant drug identifier columns updated to include the additional variable information in the format: Identifier (variable = value).

**Examples**

```
# Assuming get_env_identifiers() returns c("DrugName", "Gnumber") for drug identifiers
dt <- data.table::data.table(
  DrugName = c("DrugA", "DrugA", "DrugB"),
  Gnumber = c("G1", "G1", "G2"),
  Var1 = c(NA, "X", NA),
  Var2 = c(NA, "Y", "Z")
)
additional_vars <- c("Var1", "Var2")
dt_updated <- update_drug_name(dt, additional_vars)
# Would update DrugName and Gnumber
dt_updated
```

---

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 | <i>Update gDR synonyms for the identifier</i> |
|----------------------|-----------------------------------------------|

---

**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`    *Check that specified identifier values exist in the data.*

---

### 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

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

mae                      MultiAssayExperiment object

schema\_package      string name of the package with JSON schema files

schema\_dir\_path      path to the dir with JSON schema files

schema                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

|                   |                                                |
|-------------------|------------------------------------------------|
| <code>se</code>   | A <a href="#">SummarizedExperiment</a> object. |
| <code>name</code> | 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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