

Package ‘gDRutils’

September 15, 2024

Type Package

Title A package with helper functions for processing drug response data

Version 1.2.0

Date 2024-04-15

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

License Artistic-2.0

LazyLoad yes

Depends R (>= 4.2)

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

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

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

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

biocViews Software, Infrastructure

VignetteBuilder knitr

ByteCompile TRUE

Roxygen list(markdown = TRUE)

RoxygenNote 7.3.1

SwitchrLibrary gDRutils

DeploySubPath gDRutils

Encoding UTF-8

git_url <https://git.bioconductor.org/packages/gDRutils>

git_branch RELEASE_3_19

git_last_commit d1f7215

git_last_commit_date 2024-04-30

Repository Bioconductor 3.19

Date/Publication 2024-09-15

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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")`

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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)
```

```
.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 χ^2 value.

Value

Modified named list of fit parameters.

Examples

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

```
addClass
```

add arbitrary S3 class to an object

Description

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

Value

The same object with an added S3 class.

Examples

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

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

Description

Aggregation can only be performed on nested variables.

Usage

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

Arguments

| | |
|-----|--|
| asy | A BumpyMatrix object. |
| by | Character vector of the nested fields to aggregate by. |
| FUN | A function to use to aggregate the data. |

Value

A BumpyMatrix object aggregated by FUN.

Examples

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

apply_bumpy_function *Apply a function to every element of a bumpy matrix.*

Description

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

Usage

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

Arguments

| | |
|----------------|---|
| se | A SummarizedExperiment object with bumpy matrices. |
| FUN | A function that will be applied to each element of the matrix in assay req_assay_name. Output of the function must return a data.table. |
| req_assay_name | String of the assay name in the se that the FUN will act on. |
| out_assay_name | String of the assay name that will contain the results of the applied function. |
| parallelize | Logical indicating whether or not to parallelize the computation. |
| ... | Additional args to be passed to teh FUN. |

Value

The original se object with a new assay, out_assay_name.

Examples

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

| | |
|----------------|-----------------------|
| assert_choices | <i>assert choices</i> |
|----------------|-----------------------|

Description

assert choices

Usage

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

Arguments

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

Value

NULL

Examples

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

| | |
|----------------------------------|---------------------------------------|
| average_biological_replicates_dt | <i>Average biological replicates.</i> |
|----------------------------------|---------------------------------------|

Description

Average biological replicates on the data table side.

Usage

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

Arguments

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

Value

data.table without replicates

Examples

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

cap_xc50

Cap XC50 value.

Description

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

Usage

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

Arguments

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

Details

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

Value

Capped IC50/GR50 value.

Examples

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

convert_colData_to_json

Convert colData to JSON

Description

Convert colData to JSON format for elasticsearch indexing.

Usage

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

Arguments

| | |
|-------------|--------------------------|
| cdata | data.table of colData. |
| identifiers | charvec with identifiers |
| req_cols | charvec required columns |

Details

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

Value

JSON string capturing the cdata.

Examples

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

convert_combo_data_to_dt

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

Description

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

Usage

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

Arguments

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

Value

list of data.table(s) with combo data

Author(s)

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

Examples

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

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

Description

get combo assay names based on the field name

Usage

```
convert_combo_field_to_assay(field)
```

Arguments

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

Value

charvec

Examples

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

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

Description

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

Usage

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

Arguments

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

Details

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

Value

data.table representation of the data in assay_name.

Author(s)

Bartosz Czech bartosz.czech@contractors.roche.com

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

Description

Convert experiment metadata to JSON format for elasticsearch indexing.

Usage

```
convert_metadata_to_json(se)
```

Arguments

se SummarizedExperiment object.

Value

JSON string capturing experiment metadata.

Examples

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

convert_rowData_to_json

Convert rowData to JSON

Description

Convert rowData to JSON format for elasticsearch indexing.

Usage

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

Arguments

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

Details

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

Value

JSON string capturing the rdata.

Examples

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



```
convert_rowData_to_json(rdata, identifiers)
```

```
convert_se_assay_to_dt
```

Convert a SummarizedExperiment assay to a long data.table

Description

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

Usage

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

Arguments

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

Details

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

Value

data.table representation of the data in assay_name.

See Also

flatten

Examples

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

convert_se_to_json *Create JSON document.*

Description

Convert a SummarizedExperiment object to a JSON document.

Usage

```
convert_se_to_json(se)
```

Arguments

se SummarizedExperiment object.

Value

String representation of a JSON document.

Examples

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

```
se <- SummarizedExperiment::SummarizedExperiment(rowData = rdata,
                                                  colData = cdata)
se <- set_SE_experiment_metadata(se, md)
se <- set_SE_identifiers(se, identifiers)
convert_se_to_json(se)
```

| | |
|---------------|---|
| 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

| | |
|---------------------|--|
| <code>se</code> | A <code>SummarizedExperiment</code> object. |
| <code>fields</code> | Character vector of metadata fields to demote as nested columns. |

Details

Revert this operation using `promote_fields`.

Value

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

See Also

`promote_fields`

Examples

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

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

Description

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

Usage

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

Arguments

| | |
|--------------|---|
| data | data.table with drug-response data |
| discard_keys | a vector of keys that should be discarded |

Details

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

Value

BumpyMatrix object

Examples

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

| | |
|--------------------------------|--|
| extend_normalization_type_name | <i>extend abbreviated normalization type</i> |
|--------------------------------|--|

Description

extend abbreviated normalization type

Usage

```
extend_normalization_type_name(x)
```

Arguments

| | |
|---|--------------------------------|
| x | string with normalization type |
|---|--------------------------------|

Value

string

Examples

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

fit_curves

Fit curves

Description

Fit GR and RV curves from a data.table.

Usage

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

Arguments

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

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

Details

The df_ expects the following columns:

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

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

Value

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

Examples

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

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

flatten

Flatten a table

Description

Flatten a stacked table into a wide format.

Usage

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

Arguments

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

Details

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

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

Value

table of flattened data as defined by wide_cols.

See Also

convert_se_assay_to_dt

Examples

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

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

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

gen_synthetic_data *gen_synthetic_data*

Description

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

Usage

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

Arguments

| | |
|---|-------------------|
| m | number of drugs |
| n | number of records |

Value

list with drugs, cell_lines, raw_data and assay_data

Examples

```
gen_synthetic_data()
```

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

Description

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

Usage

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

Arguments

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

Value

numeric vector

Examples

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

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

Description

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

Usage

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


Arguments

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

Value

`charvec`

Author(s)

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

Examples

```
get_assay_names()
```

`get_combo_assay_names` *get names of combo assays*

Description

get names of combo assays

Usage

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

Arguments

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

Value

`charvec` of combo assay names.

Author(s)

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

Examples

```
get_combo_assay_names()
```

get_combo_base_assay_names
get names of combo base assays

Description

get names of combo base assays

Usage

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

Arguments

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

Value

charvec

Author(s)

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

Examples

```
get_combo_base_assay_names()
```

get_combo_col_settings
Get colorscale data for given combo assay and growth metric

Description

Get colorscale data for given combo assay and growth metric

Usage

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

Arguments

| | |
|------------|---------------|
| g_metric | growth metric |
| assay_type | assay type |

Value

list with colors, breaks and limits

Examples

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

```
get_combo_excess_field_names  
get names of combo excess fields
```

Description

get names of combo excess fields

Usage

```
get_combo_excess_field_names()
```

Value

charvec

Examples

```
get_combo_excess_field_names()
```

```
get_combo_score_assay_names  
get names of combo score assays
```

Description

get names of combo score assays

Usage

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

Arguments

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

Value

charvec

Author(s)

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

Examples

```
get_combo_score_assay_names()
```

```
get_combo_score_field_names
```

get names of combo score fields

Description

get names of combo score fields

Usage

```
get_combo_score_field_names()
```

Value

charvec

Examples

```
get_combo_score_assay_names()
```

```
get_default_identifiers
```

Get gDR default identifiers required for downstream analysis.

Description

Get gDR default identifiers required for downstream analysis.

Usage

```
get_default_identifiers()
```

Value

charvec

Examples

```
get_default_identifiers()
```

get_duplicated_rows *Helper function to find duplicated rows*

Description

Helper function to find duplicated rows

Usage

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

Arguments

x data frame
col_names character vector, columns in which duplication are searched for

Value

integer vector

Examples

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

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

Description

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

Usage

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

Arguments

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

Value

charvec

Author(s)

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

Examples

```
get_env_assay_names()
```

get_expect_one_identifiers

Get identifiers that expect only one value for each identifier.

Description

Get identifiers that expect only one value for each identifier.

Usage

```
get_expect_one_identifiers()
```

Value

charvec

Examples

```
get_expect_one_identifiers()
```

get_experiment_groups *get_experiment_groups*

Description

get experiment groups

Usage

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

Arguments

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

Value

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

Author(s)

Arkadiusz Gladki arkadiusz.gladki@contractors.roche.com

Examples

```
get_experiment_groups()
```

get_identifiers_dt *Get descriptions for identifiers*

Description

Get descriptions for identifiers

Usage

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

Arguments

k identifier key, string
get_description return descriptions only, boolean
get_example return examples only, boolean

Value

named list

Examples

```
get_identifiers_dt()
```

get_idfs_synonyms *Get gDR synonyms for the identifiers*

Description

Get gDR synonyms for the identifiers

Usage

```
get_idfs_synonyms()
```

Value

charvec

Examples

```
get_idfs_synonyms()
```

get_iso_colors *get_iso_colors*

Description

get_iso_colors

Usage

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

Arguments

normalization_type
charvec normalization_types expected in the data

Value

named charvec with iso colors

Examples

```
get_iso_colors()
```

get_MAE_identifiers *get_MAE_identifiers*

Description

get the identifiers of all SE's in the MAE

Usage

```
get_MAE_identifiers(mae)
```

Arguments

mae MultiAssayExperiment

Value

named list with identifiers for each SE

Examples

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

```
get_non_empty_assays  get_non_empty_assays
```

Description

get non empty assays

Usage

```
get_non_empty_assays(mae)
```

Arguments

mae MultiAssayExperiment object

Value

charvec with non-empty experiments

Author(s)

Arkadiusz Gladki arkadiusz.gladki@contractors.roche.com

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_synthetic_data *Get synthetic data from gDRtestData package*

Description

Get synthetic data from gDRtestData package

Usage

```
get_synthetic_data(qs)
```

Arguments

qs qs filename

Value

loaded data

Examples

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

get_testdata *get_testdata*

Description

Function to obtain data from gDRtestData and prepare for unit tests

Usage

```
get_testdata()
```

Value

list with drugs, cell_lines, raw_data and assay_data

Examples

```
get_testdata()
```

`get_testdata_codilution`
get_testdata_codilution

Description

Function to obtain data from gDRtestData and prepare for unit tests

Usage

`get_testdata_codilution()`

Value

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

Examples

`get_testdata_codilution()`

`get_testdata_combo` *get_testdata_combo*

Description

Function to obtain data from gDRtestData and prepare for unit tests

Usage

`get_testdata_combo()`

Value

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

Examples

`get_testdata_combo()`

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

Description

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

Usage

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

Arguments

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

Details

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

Value

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

Examples

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

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

Description

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

Usage

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

Arguments

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

Details

Identifiers supported by the gDR suite include:

- "barcode": String of column name containing barcode metadata
- "cellline": String of column name containing unique, machine-readable cell line identifiers
- "cellline_name": String of column name containing human-friendly cell line names
- "cellline_tissue": String of column name containing metadata on cell line tissue type
- "cellline_ref_div_time": String of column name containing reference division time for cell lines
- "cellline_parental_identifier": String of column name containing unique, machine-readable parental cell line identifiers. Used in the case of derived or engineered cell lines.
- "drug": String of column name containing unique, machine-readable drug identifiers
- "drug_name": String of column name containing human-friendly drug names
- "drug_moa": String of column name containing metadata for drug mode of action
- "duration": String of column name containing metadata on duration that cells were treated (in hours)
- "template": String of column name containing template metadata
- "untreated_tag": Character vector of entries that identify control, untreated wells
- "well_position": Character vector of column names containing metadata on well positions on a plate

Value

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

list or charvec depends on unify param

list or charvec depends on unify param

NULL

NULL

Examples

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

```
identify_unique_se_metadata_fields
      Identify unique metadata fields from a list of
      SummarizedExperiments
```

Description

Identify unique metadata fields from a list of SummarizedExperiments

Usage

```
identify_unique_se_metadata_fields(SElist)
```

Arguments

SElist named list of SummarizedExperiments

Value

character vector of unique names of metadata

Examples

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

```
is_any_exp_empty        is_any_exp_empty
```

Description

check if any experiment is empty

Usage

```
is_any_exp_empty(mae)
```

Arguments

mae MultiAssayExperiment object

Value

logical

Author(s)

Arkadiusz Gladki arkadiusz.gladki@contractors.roche.com

Examples

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

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

Description

check if experiment (SE) is empty

Usage

```
is_exp_empty(exp)
```

Arguments

exp [SummarizedExperiment](#) object.

Value

logical

Author(s)

Arkadiusz Gladki arkadiusz.gladki@contractors.roche.com

Examples

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

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

Description

check if all mae experiments are empty

Usage

```
is_mae_empty(mae)
```

Arguments

mae MultiAssayExperiment object

Value

logical

Author(s)

Arkadiusz Gladki arkadiusz.gladki@contractors.roche.com

Examples

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

| | |
|-------------|---------------------|
| logisticFit | <i>Logistic fit</i> |
|-------------|---------------------|

Description

Fit a logistic curve to drug response data.

Usage

```
logisticFit(
  concs,
  norm_values,
  std_norm_values = NA,
  x_0 = 1,
  priors = NULL,
  lower = NULL,
  range_conc = c(0.005, 5),
```

```

    force_fit = FALSE,
    pcutoff = 0.05,
    cap = 0.1,
    n_point_cutoff = 4,
    capping_fold = 5
)

```

Arguments

| | |
|-----------------|---|
| concs | concentrations that have not been transformed into log space. |
| norm_values | normalized response values (Untreated = 1). |
| std_norm_values | std of values. |
| x_0 | upper limit. Defaults to 1. For co-treatments, this value should be set to NA. |
| priors | numeric vector containing starting values for all. mean parameters in the model. Overrides any self starter function. |
| lower | numeric vector of lower limits for all parameters in a 4-param model. |
| range_conc | range of concentration for calculating AOC_range. |
| force_fit | boolean indicating whether or not to force a parameter-based fit. |
| pcutoff | numeric of pvalue significance threshold above or equal to which to use a constant fit. |
| cap | numeric value capping norm_values to stay below (x_0 + cap). |
| n_point_cutoff | integer indicating number of unique concentrations required to fit curve. |
| capping_fold | Integer value of the fold number to use for capping IC50/GR50. Default is 5. |

Details

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

The output parameter names correspond to the following definitions:

x_mean The mean of a given dose-response metric

x_AOC_range The range of the area over the curve

x_AOC The area over the GR curve or, respectively, under the relative cell count curve, averaged over the range of concentration values

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

x_max The maximum effect of the drug

ec50 The drug concentration at half-maximal effect

x_inf The asymptotic value of the sigmoidal fit to the dose-response data as concentration goes to infinity

x_0 The asymptotic metric value corresponding to a concentration of 0 for the primary drug

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

r2 The goodness of the fit

x_sd_avg The standard deviation of GR/IC

fit_type This will be given by one of the following:

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

maxlog10Concentration The highest log10 concentration

N_conc Number of unique concentrations

Value

data.table with metrics and fit parameters.

Examples

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

loop

Lapply or bplapply.

Description

Lapply or bplapply.

Usage

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

Arguments

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

Value

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

Examples

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

MAEapply

Lapply through all the experiments in MultiAssayExperiment object

Description

Lapply through all the experiments in MultiAssayExperiment object

Usage

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

Arguments

| | |
|-------|--|
| 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

Examples

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

| | |
|----------|-----------------|
| 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

Examples

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

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

Description

Merge assay data

Usage

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

Arguments

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

Value

BumpyMatrix or list with data.table + BumpyMatrix

Examples

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

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

Description

Merge metadata

Usage

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

Arguments

| | |
|-----------------|--|
| SElist | named list of SummarizedExperiments |
| metadata_fields | vector of metadata names that will be merged |

Value

list of merged metadata

Examples

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

merge_SE

Merge multiple Summarized Experiments

Description

Merge multiple Summarized Experiments

Usage

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

Arguments

SElist named list of Summarized Experiments

additional_col_name string with the name of the column that will be added to assay data for the distinction of possible duplicated metrics that can arise from multiple projects

discard_keys character vector of string that will be discarded during creating BumpyMatrix object

Value

merged SummarizedExperiment object

Examples

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

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

Description

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

Usage

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

Arguments

| | |
|--------|--|
| x | a <code>data.table</code> 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.

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

Examples

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

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

Description

Predict a concentration for a given efficacy with fit parameters.

Usage

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

Arguments

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

Details

The inverse of this function is `predict_efficacy_from_conc`.

Value

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

See Also

`predict_efficacy_from_conc` `.calculate_x50`

Examples

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

predict_efficacy_from_conc

Predict efficacy values given fit parameters and a concentration.

Description

Predict efficacy values given fit parameters and a concentration.

Usage

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

Arguments

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

Details

The inverse of this function is `predict_conc_from_efficacy`.

Value

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

See Also

`predict_conc_from_efficacy`

Examples

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

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

Description

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

Usage

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

Arguments

x character vector of names to prettify.

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

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

Details

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

Value

character vector of prettified names.

Examples

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

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

Description

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

Usage

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

Arguments

| | |
|--------|--|
| se | SummarizedExperiment object. |
| fields | Character vector of nested fields in a BumpyMatrix object to promote to metadata fields of a se. |
| MARGIN | Numeric of values 1 or 2 indicating whether to promote fields to rows or columns respectively. |

Details

Revert this operation using demote_fields.

Value

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

See Also

demote_fields

Examples

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

| | |
|----------------|-----------------------|
| 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]])
```

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"))
```

| | |
|-------------------------|--|
| set_constant_fit_params | |
|-------------------------|--|

Set fit parameters for a constant fit.

Description

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

Usage

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

Arguments

| | |
|-----------------|--|
| out | Named list of fit parameters. |
| mean_norm_value | Numeric value that be used to set all parameters that can be calculated from the mean. |

Value

Modified named list of fit parameters.

Examples

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

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

Description

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

Usage

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

Arguments

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

Details

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

Value

se with added metadata.

Examples

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

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

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

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

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

shorten_normalization_type_name
shorten normalization type

Description

shorten normalization type

Usage

```
shorten_normalization_type_name(x)
```

Arguments

x string with normalization type

Value

shortened string representing the normalization type

Examples

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

```
split_SE_components    split_SE_components
```

Description

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

Usage

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

Arguments

df_ `data.table` with drug-response data

nested_keys character vector of keys to exclude from the row or column metadata, and to instead nest within an element of the matrix. See details.

combine_on 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(cldid = "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.

```
update_env_idfs_from_mae
```

Update environment identifiers from MAE object identifiers

Description

Update environment identifiers from MAE object identifiers

Usage

```
update_env_idfs_from_mae(mae_idfs)
```

Arguments

mae_idfs A list containing MAE identifiers

Value

NULL

Examples

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

```
update_idfs_synonyms    Update gDR synonyms for the identifier
```

Description

Update gDR synonyms for the identifier

Usage

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

Arguments

data list of charvec with identifiers data
dict list with dictionary

Value

list

Examples

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

validate_dimnames *Validate dimnames*

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

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

Details

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

Value

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

Examples

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

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

Description

Validate JSON describing an object against a schema.

Usage

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

Arguments

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

Details

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

Value

Boolean of whether or not JSON successfully validated.

Examples

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

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

Description

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

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

Usage

```
validate_MAE(mae)
```

Arguments

mae MultiAssayExperiment object produced by the gDR pipeline

Value

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

Author(s)

Bartosz Czech bartosz.czech@contractors.roche.com

Examples

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

`validate_mae_with_schema`*Validate MAE against a schema.*

Description

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

Usage

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

Arguments

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

Value

Boolean of whether or not mae is valid

Examples

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

`validate_SE`*Validate SummarizedExperiment object*

Description

Function validates correctness of SE by checking multiple cases:

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

Usage

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

Arguments

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

Value

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

Examples

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

```
validate_se_assay_name
```

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

Description

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

Usage

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

Arguments

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

Value

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

Examples

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

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