Package 'QurvE'

January 26, 2024

Title Robust and User-Friendly Analysis of Growth and Fluorescence Curves

Version 1.1.1

Description High-throughput analysis of growth curves and fluorescence data using three methods: linear regression, growth model fitting, and smooth spline fit. Analysis of dose-response relationships via smoothing splines or dose-response models. Complete data analysis workflows can be executed in a single step via user-friendly wrapper functions. The results of these workflows are summarized in detailed reports as well as intuitively navigable 'R' data containers. A 'shiny' application provides access to all features without requiring any programming knowledge. The package is described in further detail in Wirth et al. (2023) <doi:10.1038/s41596-023-00850-7>.

License GPL (>= 3)

URL https://github.com/NicWir/QurvE, https://nicwir.github.io/QurvE/

BugReports https://github.com/NicWir/QurvE/issues

Depends dplyr, methods, R (>= 4.0), stringr, tidyr

Imports doParallel, drc, DT, foreach, ggh4x, ggnewscale, ggplot2, ggpubr, kableExtra, knitr, labeling, magrittr, minpack.lm, plyr, purrr, RColorBrewer, readxl, rmarkdown, scales, shiny, stats, utils

Suggests bookdown, Cairo, htmltools, plotrix, prettydoc, rlang, shinyBS, shinycssloaders, shinyFiles, shinyjs, shinysurveys, shinythemes, testthat (>= 3.0.0), tibble, tinytex

VignetteBuilder knitr

Encoding UTF-8

NeedsCompilation yes

RoxygenNote 7.2.3

Collate 'QurvE-package.R' 'control_functions.R' 'data_parsers.R' 'dose-response-analysis.R' 'fluorescence_plots.R' 'fluorescence_summaries.R' 'fluorescence_workflows.R'

'group_tables.R' 'growth_plots.R' 'growth_summaries.R'
'growth_workflows.R' 'linear_fits.R' 'nonparametric_fits.R'
'parametric_fits.R' 'utils.R' 'report_functions.R'
'shiny_app_functions.R'

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Mark Heckmann [ctb] (Creator of the 'zipFastener' function; source:
https://ryouready.wordpress.com/2009/03/27/r-zip-fastener-for-two-data-frames-combining-
rows-or-columns-of-two-dataframes-in-an-alternating-manner/),
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functions are used to display function help pages within the shiny
app.)

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Repository CRAN

Date/Publication 2024-01-26 12:40:14 UTC

R topics documented:

`biosensor.eq` *Internal function used to fit a biosensor response model with* `nlsLM`

Description

Calculates the values of biosensor response model for given time points and response parameters.

Usage

```
biosensor.eq(x, y.min, y.max, K, n)
```

Arguments

`x`	A vector of concentration values
`y.min`	The minimum fluorescence value
`y.max`	The maximum fluorescence value
`K`	Sensitivity parameter
`n`	Cooperativity parameter

Value

A vector of fluorescence values

References

Meyer, A.J., Segall-Shapiro, T.H., Glassey, E. et al. *Escherichia coli "Marionette" strains with 12 highly optimized small-molecule sensors.* Nat Chem Biol 15, 196–204 (2019). DOI: 10.1038/s41589-018-0168-3

Examples

```
n <- seq(1:10)
conc <- rev(10*(1/2)^n)
fit <- biosensor.eq(conc, 300, 82000, 0.85, 2)
```

`export_RData` *Export an R object as .RData file*

Description

Export an R object as .RData file

Usage

```
export_RData(object, out.dir = tempdir(), out.nm = class(object))
```

Arguments

`object`	An R object.
`out.dir`	The path to the output directory. Default: the working directory
`out.nm`	The output filename (with or without '.RData' ending). Default: the class of `object` followed by '.RData'.

Value

`NULL`

Examples

```
if(interactive()){
df <- data.frame('A' = seq(1:10), 'B' = rev(seq(1:10)))

export_RData(df)
}
```

export_Table *Export a tabular object as tab-separated .txt file*

Description

Export a tabular object as tab-separated .txt file

Usage

```
export_Table(table, out.dir = tempdir(), out.nm = deparse(substitute(table)))
```

Arguments

table	A tabular R object (dataframe, matrix, array)
out.dir	The path to the output directory. Default: the working directory
out.nm	The output filename (with or without '.txt' ending). Default: the name of table followed by '.txt'.

Value

NULL

Examples

```
if(interactive()){
df <- data.frame('A' = seq(1:10), 'B' = rev(seq(1:10)))

export_Table(df)
}
```

fl.control *Create a* fl.control *object.*

Description

A fl.control object is required to perform various computations on fluorescence data stored within grodata objects (created with read_data or parse_data). A fl.control object is created automatically as part of fl.workflow.

Usage

```
fl.control(
  fit.opt = c("l", "s"),
  x_type = c("growth", "time"),
  norm_fl = TRUE,
  t0 = 0,
  tmax = NA,
  min.growth = NA,
  max.growth = NA,
  log.x.lin = FALSE,
  log.x.spline = FALSE,
  log.y.lin = FALSE,
  log.y.spline = FALSE,
  lin.h = NULL,
  lin.R2 = 0.97,
  lin.RSD = 0.05,
  lin.dY = 0.05,
  dr.parameter = "max_slope.spline",
  dr.method = c("model", "spline"),
  dr.have.atleast = 5,
  smooth.dr = NULL,
  log.x.dr = FALSE,
  log.y.dr = FALSE,
  nboot.dr = 0,
  biphasic = FALSE,
  interactive = FALSE,
  nboot.fl = 0,
  smooth.fl = 0.75,
  growth.thresh = 1.5,
  suppress.messages = FALSE,
  neg.nan.act = FALSE,
  clean.bootstrap = TRUE
)
```

Arguments

`fit.opt`	(Character or vector of strings) Indicates whether the program should perform a linear regression (`'l'`) and/or spline fit (`'s'`). Default: `fit.opt = c('l', 's')`.
`x_type`	(Character) Which data type shall be used as independent variable? Options are `'growth'` and `'time'`.
`norm_fl`	(Logical) use normalized (to growth) fluorescence data in fits. Has an effect only when `x_type = 'time'`
`t0`	(Numeric) Minimum time value considered for linear and spline fits (if `x_type = 'time'`).
`tmax`	(Numeric) Maximum time value considered for linear and spline fits (if `x_type = 'time'`)..

`min.growth` (Numeric) Indicate whether only values above a certain threshold should be considered for linear regressions or spline fits (if `x_type = 'growth'`).

`max.growth` (Numeric) Indicate whether only growth values below a certain threshold should be considered for linear regressions or spline fits (if `x_type = 'growth'`).

`log.x.lin` (Logical) Indicates whether *ln(x+1)* should be applied to the independent variable for *linear* fits. Default: `FALSE`.

`log.x.spline` (Logical) Indicates whether *ln(x+1)* should be applied to the independent variable for *spline* fits. Default: `FALSE`.

`log.y.lin` (Logical) Indicates whether *ln(y/y0)* should be applied to the fluorescence data for *linear* fits. Default: `FALSE`

`log.y.spline` (Logical) Indicates whether *ln(y/y0)* should be applied to the fluorescence data for *spline* fits. Default: `FALSE`

`lin.h` (Numeric) Manually define the size of the sliding window used in `flFitLinear`. If `NULL`, h is calculated for each samples based on the number of measurements in the fluorescence increase phase of the plot.

`lin.R2` (Numeric) R^2 threshold for `flFitLinear`.

`lin.RSD` (Numeric) Relative standard deviation (RSD) threshold for the calculated slope in `flFitLinear`.

`lin.dY` (Numeric) Threshold for the minimum fraction of growth increase a linear regression window should cover. Default: 0.05 (5%).

`dr.parameter` (Character or numeric) The response parameter in the output table to be used for creating a dose response curve. See `fl.drFit` for further details. Default: `'max_slope.spline'`, which represents the maximum slope of the spline fit Typical options include: `'max_slope.linfit'`, `'dY.linfit'`, `'max_slope.spline'`, and `'dY.spline'`.

`dr.method` (Character) Perform either a smooth spline fit on response parameter vs. concentration data (`'spline'`) or fit a biosensor response model with `'model'` (proposed by Meyer et al., 2019).

`dr.have.atleast` (Numeric) Minimum number of different values for the response parameter one should have for estimating a dose response curve. Note: All fit procedures require at least six unique values. Default: `6`.

`smooth.dr` (Numeric) Smoothing parameter used in the spline fit by smooth.spline during dose response curve estimation. Usually (not necessesary) in (0; 1]. See `smooth.spline` for further details. Default: `NULL`.

`log.x.dr` (Logical) Indicates whether `ln(x+1)` should be applied to the concentration data of the dose response curves. Default: `FALSE`.

`log.y.dr` (Logical) Indicates whether `ln(y+1)` should be applied to the response data of the dose response curves. Default: `FALSE`.

`nboot.dr` (Numeric) Defines the number of bootstrap samples for EC50 estimation. Use `nboot.dr = 0` to disable bootstrapping. Default: `0`.

`biphasic` (Logical) Shall `flFitLinear` and `flFitSpline` try to extract fluorescence parameters for two different phases (as observed with, e.g., regulator-promoter systems with varying response in different growth stages) (`TRUE`) or not (`FALSE`)?

`interactive` (Logical) Controls whether the fit for each sample and method is controlled manually by the user. If `TRUE`, each fit is visualized in the *Plots* pane and the user can adjust fitting parameters and confirm the reliability of each fit per sample. Default: `TRUE`.

`nboot.fl` (Numeric) Number of bootstrap samples used for nonparametric curve fitting with `flBootSpline`. Use `nboot.fl = 0` to disable the bootstrap. Default: `0`

`smooth.fl` (Numeric) Parameter describing the smoothness of the spline fit; usually (not necessary) within (0;1]. `smooth.gc=NULL` causes the program to query an optimal value via cross validation techniques. Especially for datasets with few data points the option `NULL` might cause a too small smoothing parameter. This can result a too tight fit that is susceptible to measurement errors (thus overestimating slopes) or produce an error in `smooth.spline` or lead to overfitting. The usage of a fixed value is recommended for reproducible results across samples. See `smooth.spline` for further details. Default: `0.55`

`growth.thresh` (Numeric) Define a threshold for growth. Only if any growth value in a sample is greater than `growth.thresh` (default: 1.5) times the start growth, further computations are performed. Else, a message is returned.

`suppress.messages` (Logical) Indicates whether messages (information about current fluorescence curve, EC50 values etc.) should be displayed (`FALSE`) or not (`TRUE`). This option is meant to speed up the high-throughput processing data. Note: warnings are still displayed. Default: `FALSE`.

`neg.nan.act` (Logical) Indicates whether the program should stop when negative fluorescence values or NA values appear (`TRUE`). Otherwise, the program removes these values silently (`FALSE`). Improper values may be caused by incorrect data or input errors. Default: `FALSE`.

`clean.bootstrap` (Logical) Determines if negative values which occur during bootstrap should be removed (`TRUE`) or kept (`FALSE`). Note: Infinite values are always removed. Default: `TRUE`.

Value

Generates a list with all arguments described above as entries.

References

Meyer, A.J., Segall-Shapiro, T.H., Glassey, E. et al. *Escherichia coli "Marionette" strains with 12 highly optimized small-molecule sensors.* Nat Chem Biol 15, 196–204 (2019). DOI: 10.1038/s41589-018-0168-3

Examples

```
# default option
control_default <- fl.control()
# user defined
control_manual <- fl.control(fit.opt = c('s'),
                             smooth.fl = 0.6,
```

```
                    x_type = 'time',
                    t0 = 2)
```

`fl.drFit` *Fit a biosensor model (Meyer et al., 2019) to response vs. concentration data*

Description

Fit a biosensor model (Meyer et al., 2019) to response vs. concentration data

Usage

```
fl.drFit(
  flTable,
  control = fl.control(dr.method = "model", dr.parameter = "max_slope.spline")
)
```

Arguments

`flTable`	A dataframe containing the data for the dose-response model estimation. Such table of class `flTable` can be obtained by running `flFit` with `dr.method = 'model'` as argument in the `fl.control` object.
`control`	A `fl.control` object created with `fl.control`, defining relevant fitting options.
`dr.method`	(Character) Perform either a smooth spline fit on response parameter vs. concentration data (`'spline'`) or fit a biosensor response model with `'model'` (proposed by Meyer et al., 2019).
`dr.parameter`	(Character or numeric) The response parameter in the output table to be used for creating a dose response curve. See `fl.drFit` for further details. Default: `'max_slope.spline'`, which represents the maximum slope of the spline fit Typical options include: `'max_slope.linfit'`, `'dY.linfit'`, `'max_slope.spline'`, and `'dY.spline'`.

Details

Common response parameters used in dose-response analysis:Linear fit:- max_slope.linfit: Fluorescence increase rate- lambda.linfit: Lag time- dY.linfit: Maximum Fluorescence - Minimum Fluorescence- A.linfit: Maximum fluorescenceSpline fit:- max_slope.spline: Fluorescence increase rate- lambda.spline: Lag time- dY.spline: Maximum Fluorescence - Minimum Fluorescence- A.spline: Maximum fluorescence- integral.spline: IntegralParametric fit:- max_slope.model: Fluorescence increase rate- lambda.model: Lag time- dY.model: Maximum Fluorescence - Minimum Fluorescence- A.model: Maximum fluorescence- integral.model: Integral'

Value

An object of class drFit.

raw.data	Data that passed to the function as flTable.
drTable	Dataframe containing condition identifiers, fit options, and results of the dose-response analysis.
drFittedModels	List of all drFitModel objects generated by the call of fl.drFitModel for each distinct experiment.
control	Object of class fl.control created with the call of fl.control.

References

Meyer, A.J., Segall-Shapiro, T.H., Glassey, E. et al. *Escherichia coli "Marionette" strains with 12 highly optimized small-molecule sensors.* Nat Chem Biol 15, 196–204 (2019). DOI: 10.1038/s41589-018-0168-3

Examples

```
# Load example dataset
input <- read_data(data.fl = system.file('lac_promoters_fluorescence.txt', package = 'QurvE'),
                   csvsep.fl = "\t")

# Run fluorescence curve analysis workflow
fitres <- flFit(fl_data = input$fluorescence,
                time = input$time,
                parallelize = FALSE,
                control = fl.control(x_type = 'time', norm_fl = FALSE,
                                     suppress.messages = TRUE))

# Perform dose-response analysis
drFit <- fl.drFit(flTable = fitres$flTable,
                  control = fl.control(dr.method = 'model',
                                       dr.parameter = 'max_slope.linfit'))

# Inspect results
summary(drFit)
plot(drFit)
```

---

fl.drFitModel *Perform a biosensor model fit on response vs. concentration data of a single sample.*

Description

fl.drFitModel fits the biosensor model proposed by Meyer et al. (2019) to the provided response (e.g., max_slope.spline vs. concentration data to determine the leakiness, sensitivity, induction fold-change, and cooperativity.

Usage

```
fl.drFitModel(conc, test, drID = "undefined", control = fl.control())
```

Arguments

conc	Vector of concentration values.
test	Vector of response parameter values of the same length as conc.
drID	(Character) The name of the analyzed condition
control	A fl.control object created with fl.control, defining relevant fitting options.

Value

A drFitFLModel object.

raw.conc	Raw data provided to the function as conc.
raw.test	Raw data for the response parameter provided to the function as test.
drID	(Character) Identifies the tested condition
fit.conc	Fitted concentration values.
fit.test	Fitted response values.
model	nls object generated by the nlsLM function.
parameters	List of parameters estimated from dose response curve fit.

- yEC50: Response value related to EC50.
- y.min: Minimum fluorescence ('leakiness', if lowest concentration is 0).
- y.max: Maximum fluorescence.
- fc: Fold change (y.max divided by y.min).
- K: Concentration at half-maximal response ('sensitivity').
- n: Cooperativity.
- yEC50.orig: Response value for EC50 in original scale, if a transformation was applied.
- K.orig: K in original scale, if a transformation was applied.
- test.nm: Test identifier extracted from test.

fitFlag	(Logical) Indicates whether a spline could fitted successfully to data.
reliable	(Logical) Indicates whether the performed fit is reliable (to be set manually).
control	Object of class fl.control created with the call of fl.control.

Use plot.drFitModel to visualize the model fit.

References

Meyer, A.J., Segall-Shapiro, T.H., Glassey, E. et al. *Escherichia coli "Marionette" strains with 12 highly optimized small-molecule sensors.* Nat Chem Biol 15, 196–204 (2019). DOI: 10.1038/s41589-018-0168-3

Examples

```
# Create concentration values via a serial dilution
conc <- c(0, rev(unlist(lapply(1:18, function(x) 10*(2/3)^x))),10)

# Simulate response values via biosensor equation
response <- biosensor.eq(conc, y.min = 110, y.max = 6000, K = 0.5, n = 2) +
            0.01*6000*rnorm(10)

# Perform fit
TestRun <- fl.drFitModel(conc, response, drID = 'test', control = fl.control())

print(summary(TestRun))
plot(TestRun)
```

`fl.report` *Create a PDF and HTML report with results from a fluorescence analysis workflow*

Description

`fl.report` requires a `flFitRes` object and creates a report in PDF and HTML format that summarizes all results obtained.

Usage

```
fl.report(
  flFitRes,
  out.dir = tempdir(),
  out.nm = NULL,
  ec50 = FALSE,
  format = c("pdf", "html"),
  export = FALSE,
  parallelize = TRUE,
  ...
)
```

Arguments

`flFitRes`	A `grofit` object created with `fl.workflow`.
`out.dir`	(Character) The path or name of the folder in which the report files are created. If `NULL`, the folder will be named with a combination of 'Report.fluorescence_' and the current date and time.
`out.nm`	Character or `NULL` Define the name of the report files. If `NULL`, the files will be named with a combination of 'FluorescenceReport_' and the current date and time.
`ec50`	(Logical) Display results of dose-response analysis (`TRUE`) or not (`FALSE`).

format (Character) Define the file format for the report, PDF ('pdf') and/or HTML ('html'). Default: (c('pdf', 'html'))

export (Logical) Shall all plots generated in the report be exported as individual PDF and PNG files TRUE or not FALSE?

parallelize (Logical) Create plots using all but one available processor cores (TRUE) or only a single core (FALSE).

... Further arguments passed to create a report. Currently supported:

- mean.grp: Define groups to combine into common plots in the report based on sample identifiers. Partial matches with sample/group names are accepted. Can be 'all', a vector of strings, or a list of string vectors. Note: The maximum number of sample groups (with unique condition/concentration indicators) is 50. If you have more than 50 groups, option 'all' will produce the error ! Insufficient values in manual scale. [Number] needed but only 50 provided.
- mean.conc: Define concentrations to combine into common plots in the report. Can be a numeric vector, or a list of numeric vectors.

Details

The template .Rmd file used within this function can be found within the QurvE package installation directory.

Value

NULL

Examples

```
# load example dataset
## Not run:
input <- read_data(data.growth = system.file("lac_promoters_growth.txt", package = "QurvE"),
              data.fl = system.file("lac_promoters_fluorescence.txt", package = "QurvE"),
                   csvsep = "\t",
                   csvsep.fl = "\t")

# Run workflow
res <- fl.workflow(grodata = input, ec50 = FALSE, fit.opt = 's',
                   x_type = 'time', norm_fl = TRUE,
                   dr.parameter = 'max_slope.spline',
                   suppress.messages = TRUE,
                   parallelize = FALSE)

fl.report(res, out.dir = tempdir(), parallelize = FALSE)

## End(Not run)
```

`fl.workflow` *Run a complete fluorescence curve analysis and dose-reponse analysis workflow.*

Description

`fl.workflow` runs `fl.control` to create a `fl.control` object and then performs all computational fitting operations based on the user input. Finally, if desired, a final report is created in PDF or HTML format that summarizes all results obtained.

Usage

```
fl.workflow(
  grodata = NULL,
  time = NULL,
  growth = NULL,
  fl_data = NULL,
  ec50 = TRUE,
  mean.grp = NA,
  mean.conc = NA,
  fit.opt = c("l", "s"),
  x_type = c("growth", "time"),
  norm_fl = TRUE,
  t0 = 0,
  tmax = NA,
  min.growth = 0,
  max.growth = NA,
  log.x.lin = FALSE,
  log.x.spline = FALSE,
  log.y.lin = FALSE,
  log.y.spline = FALSE,
  lin.h = NULL,
  lin.R2 = 0.97,
  lin.RSD = 0.07,
  lin.dY = 0.05,
  biphasic = FALSE,
  interactive = FALSE,
  dr.parameter = "max_slope.spline",
  dr.method = c("model", "spline"),
  dr.have.atleast = 5,
  smooth.dr = NULL,
  log.x.dr = FALSE,
  log.y.dr = FALSE,
  nboot.dr = 0,
  nboot.fl = 0,
  smooth.fl = 0.75,
  growth.thresh = 1.5,
```

```
  suppress.messages = FALSE,
  neg.nan.act = FALSE,
  clean.bootstrap = TRUE,
  report = NULL,
  out.dir = NULL,
  out.nm = NULL,
  export.fig = FALSE,
  export.res = FALSE,
  parallelize = TRUE,
  ...
)
```

Arguments

grodata	A grodata object created with read_data or parse_data, containing fluorescence data and data for the independent variable (i.e., time or growth).
time	(optional) A matrix containing time values for each sample (if a fl_data dataframe is provided as separate argument).
growth	(optional) A dataframe containing growth data (if a fl_data matrix is provided as separate argument).
fl_data	(optional) A dataframe containing fluorescence data (if a time matrix or growth dataframe is provided as separate argument).
ec50	(Logical) Perform dose-response analysis (TRUE) or not (FALSE).
mean.grp	("all", a string vector, or a list of string vectors) Define groups to combine into common plots in the final report based on sample identifiers (if report == TRUE). Partial matches with sample/group names are accepted. Note: The maximum number of sample groups (with unique condition/concentration indicators) is 50. If you have more than 50 groups, option "all" will produce the error ! Insufficient values in manual scale. [Number] needed but only 50 provided.
mean.conc	(A numeric vector, or a list of numeric vectors) Define concentrations to combine into common plots in the final report (if report == TRUE).
fit.opt	(Character or character vector) Indicates whether the program should perform a linear regression ("l"), model fit ("m"), spline fit ("s"), or all ("a"). Combinations can be freely chosen by providing a character vector, e.g. fit.opt = c("l", "s") Default: fit.opt = c("l", "s").
x_type	(Character) Which data type shall be used as independent variable? Options are 'growth' and 'time'.
norm_fl	(Logical) use normalized (to growth) fluorescence data in fits. Has an effect only when x_type = 'time'
t0	(Numeric) Minimum time value considered for linear and spline fits (if x_type = 'time').
tmax	(Numeric) Maximum time value considered for linear and spline fits (if x_type = 'time')..
min.growth	(Numeric) Indicate whether only values above a certain threshold should be considered for linear regressions or spline fits (if x_type = 'growth').

`max.growth` (Numeric) Indicate whether only growth values below a certain threshold should be considered for linear regressions or spline fits (if `x_type = 'growth'`).

`log.x.lin` (Logical) Indicates whether *ln(x+1)* should be applied to the independent variable for *linear* fits. Default: `FALSE`.

`log.x.spline` (Logical) Indicates whether *ln(x+1)* should be applied to the independent variable for *spline* fits. Default: `FALSE`.

`log.y.lin` (Logical) Indicates whether *ln(y/y0)* should be applied to the fluorescence data for *linear* fits. Default: `FALSE`

`log.y.spline` (Logical) Indicates whether *ln(y/y0)* should be applied to the fluorescence data for *spline* fits. Default: `FALSE`

`lin.h` (Numeric) Manually define the size of the sliding window used in `flFitLinear`. If `NULL`, h is calculated for each samples based on the number of measurements in the fluorescence increase phase of the plot.

`lin.R2` (Numeric) R^2 threshold for `flFitLinear`.

`lin.RSD` (Numeric) Relative standard deviation (RSD) threshold for the calculated slope in `flFitLinear`.

`lin.dY` (Numeric) Threshold for the minimum fraction of growth increase a linear regression window should cover. Default: 0.05 (5%).

`biphasic` (Logical) Shall `flFitLinear` and `flFitSpline` try to extract fluorescence parameters for two different phases (as observed with, e.g., regulator-promoter systems with varying response in different growth stages) (`TRUE`) or not (`FALSE`)?

`interactive` (Logical) Controls whether the fit for each sample and method is controlled manually by the user. If `TRUE`, each fit is visualized in the *Plots* pane and the user can adjust fitting parameters and confirm the reliability of each fit per sample. Default: `TRUE`.

`dr.parameter` (Character or numeric) The response parameter in the output table to be used for creating a dose response curve. See `fl.drFit` for further details. Default: `"max_slope.spline"`, which represents the maximum slope of the spline fit Typical options include: `"max_slope.linfit"`, `"dY.linfit"`, `"max_slope.spline"`, and `"dY.spline"`.

`dr.method` (Character) Perform either a smooth spline fit on response parameter vs. concentration data (`"spline"`) or fit a biosensor response model (proposed by Meyer et al., 2019).

`dr.have.atleast` (Numeric) Minimum number of different values for the response parameter one should have for estimating a dose response curve. Note: All fit procedures require at least six unique values. Default: `6`.

`smooth.dr` (Numeric) Smoothing parameter used in the spline fit by smooth.spline during dose response curve estimation. Usually (not necessesary) in (0; 1]. See `smooth.spline` for further details. Default: `NULL`.

`log.x.dr` (Logical) Indicates whether `ln(x+1)` should be applied to the concentration data of the dose response curves. Default: `FALSE`.

`log.y.dr` (Logical) Indicates whether `ln(y+1)` should be applied to the response data of the dose response curves. Default: `FALSE`.

`nboot.dr` (Numeric) Defines the number of bootstrap samples for EC50 estimation. Use `nboot.dr = 0` to disable bootstrapping. Default: `0`.

`nboot.fl` (Numeric) Number of bootstrap samples used for nonparametric curve fitting with `flBootSpline`. Use `nboot.fl = 0` to disable the bootstrap. Default: `0`

`smooth.fl` (Numeric) Parameter describing the smoothness of the spline fit; usually (not necessary) within (0;1]. `smooth.gc=NULL` causes the program to query an optimal value via cross validation techniques. Especially for datasets with few data points the option `NULL` might cause a too small smoothing parameter. This can result a too tight fit that is susceptible to measurement errors (thus overestimating slopes) or produce an error in `smooth.spline` or lead to overfitting. The usage of a fixed value is recommended for reproducible results across samples. See `smooth.spline` for further details. Default: `0.55`

`growth.thresh` (Numeric) Define a threshold for growth. Only if any growth value in a sample is greater than `growth.thresh` (default: 1.5) times the start growth, further computations are performed. Else, a message is returned.

`suppress.messages` (Logical) Indicates whether messages (information about current fluorescence curve, EC50 values etc.) should be displayed (`FALSE`) or not (`TRUE`). This option is meant to speed up the high-throughput processing data. Note: warnings are still displayed. Default: `FALSE`.

`neg.nan.act` (Logical) Indicates whether the program should stop when negative fluorescence values or NA values appear (`TRUE`). Otherwise, the program removes these values silently (`FALSE`). Improper values may be caused by incorrect data or input errors. Default: `FALSE`.

`clean.bootstrap` (Logical) Determines if negative values which occur during bootstrap should be removed (`TRUE`) or kept (`FALSE`). Note: Infinite values are always removed. Default: `TRUE`.

`report` (Character or NULL) Create a PDF (`'pdf'`) and/or HTML (`'html'`) report after running all computations. Define `NULL` if no report should be created. Default: (`c('pdf', 'html')`)

`out.dir` Character or `NULL` Define the name of a folder in which all result files (tables and reports) are stored. If `NULL`, the folder will be named with a combination of "FluorescenceResults_" and the current date and time.

`out.nm` Character or `NULL` Define the name of the report files. If `NULL`, the files will be named with a combination of "FluorescenceReport_" and the current date and time.

`export.fig` (Logical) Export all figures created in the report as separate PNG and PDF files (`TRUE`) or not (`FALSE`). Only effective if `report = TRUE`.

`export.res` (Logical) Create tab-separated TXT files containing calculated parameters and dose-response analysis results as well as an .RData file for the resulting `flFitRes` object.

`parallelize` Run linear fits and bootstrapping operations in parallel using all but one available processor cores

`...` Further arguments passed to the shiny app.

Value

A `flFitRes` object that contains all computation results, compatible with various plotting functions of the QurvE package and with `fl.report`.

`time`	Raw time matrix passed to the function as `time` (if no `grofit` object is provided. Else, extracted from `grofit`).
`data`	Raw data dataframe passed to the function as `grodata`.
`flFit`	`flFit` object created with the call of `flFit` on fluorescence data.
`drFit`	`drFit` or `drFitfl` object created with the call of `growth.drFit` or `fl.drFit` for fluorescence data (based on the `dr.method` argument in `control`; see `fl.control`).
`expdesign`	Experimental design table inherited from `grodata` or created from the identifier columns (columns 1-3) in `data`.
`control`	Object of class `fl.control` created with the call of `fl.control`.

Examples

```
# load example dataset
input <- read_data(data.growth = system.file("lac_promoters_growth.txt", package = "QurvE"),
              data.fl = system.file("lac_promoters_fluorescence.txt", package = "QurvE"),
                   csvsep = "\t",
                   csvsep.fl = "\t")

# Run workflow
res <- fl.workflow(grodata = input, ec50 = FALSE, fit.opt = "s",
                   x_type = "time", norm_fl = TRUE,
                   dr.parameter = "max_slope.spline",
                   suppress.messages = TRUE,
                   parallelize = FALSE)

plot(res, data.type = "raw", legend.ncol = 3, basesize = 15)
```

`flBootSpline` *flBootSpline: Function to generate a bootstrap*

Description

`fl.gcBootSpline` resamples the fluorescence-'x' value pairs in a dataset with replacement and performs a spline fit for each bootstrap sample.

Usage

```
flBootSpline(
  time = NULL,
  growth = NULL,
  fl_data,
  ID = "undefined",
  control = fl.control()
)
```

Arguments

time	Vector of the independent variable: time (if x_type = 'time' in fl.control object.
growth	Vector of the independent variable: growth (if x_type = 'growth' in fl.control object.
fl_data	Vector of dependent variable: fluorescence.
ID	(Character) The name of the analyzed sample.
control	A fl.control object created with fl.control, defining relevant fitting options.

Value

A gcBootSpline object containing a distribution of fluorescence parameters and a flFitSpline object for each bootstrap sample. Use plot.gcBootSpline to visualize all bootstrapping splines as well as the distribution of physiological parameters.

raw.x	Raw time values provided to the function as time.
raw.fl	Raw growth data provided to the function as data.
ID	(Character) Identifies the tested sample.
boot.x	Table of time values per column, resulting from each spline fit of the bootstrap.
boot.fl	Table of growth values per column, resulting from each spline fit of the bootstrap.
boot.flSpline	List of flFitSpline object, created by flFitSpline for each resample of the bootstrap.
lambda	Vector of estimated lambda (lag time) values from each bootstrap entry.
max_slope	Vector of estimated max_slope (maximum slope) values from each bootstrap entry.
A	Vector of estimated A (maximum fluorescence) values from each bootstrap entry.
integral	Vector of estimated integral values from each bootstrap entry.
bootFlag	(Logical) Indicates the success of the bootstrapping operation.
control	Object of class fl.control containing list of options passed to the function as control.

See Also

Other fluorescence fitting functions: flFitSpline(), flFit()

Examples

```
# load example dataset
input <- read_data(data.growth = system.file("lac_promoters_growth.txt", package = "QurvE"),
              data.fl = system.file("lac_promoters_fluorescence.txt", package = "QurvE"),
                   csvsep = "\t",
                   csvsep.fl = "\t")
```

```
# Extract time and normalized fluorescence data for single sample
time <- input$time[4,]
data <- input$norm.fluorescence[4,-(1:3)] # Remove identifier columns

# Perform linear fit
TestFit <- flBootSpline(time = time,
                        fl_data = data,
                        ID = 'TestFit',
                        control = fl.control(fit.opt = 's', x_type = 'time',
                        nboot.fl = 50))

plot(TestFit, combine = TRUE, lwd = 0.5)
```

`flFit` *Perform a fluorescence curve analysis on all samples in the provided dataset.*

Description

`flFit` performs all computational fluorescence fitting operations based on the user input.

Usage

```
flFit(
  fl_data,
  time = NULL,
  growth = NULL,
  control = fl.control(),
  parallelize = TRUE,
  ...
)
```

Arguments

`fl_data`	Either... 1. a `grodata` object created with `read_data` or `parse_data`, 2. a list containing a `'time'` matrix (for x_type == "time") or `'growth'` dataframe (for x_type == "growth") and a `'fluorescence'` dataframes, or 3. a dataframe containing (normalized) fluorescence values (if a `time` matrix or `growth` dataframe is provided as separate argument).
`time`	(optional) A matrix containing time values for each sample.
`growth`	(optional) A dataframe containing growth values for each sample and sample identifiers in the first three columns.
`control`	A `fl.control` object created with `fl.control`, defining relevant fitting options.

parallelize	Run linear fits and bootstrapping operations in parallel using all but one available processor cores
...	Further arguments passed to the shiny app.

Details

Common response parameters used in dose-response analysis:Linear fit:- max_slope.linfit: Fluorescence increase rate- lambda.linfit: Lag time- dY.linfit: Maximum Fluorescence - Minimum Fluorescence- A.linfit: Maximum fluorescenceSpline fit:- max_slope.spline: Fluorescence increase rate- lambda.spline: Lag time- dY.spline: Maximum Fluorescence - Minimum Fluorescence- A.spline: Maximum fluorescence- integral.spline: IntegralParametric fit:- max_slope.model: Fluorescence increase rate- lambda.model: Lag time- dY.model: Maximum Fluorescence - Minimum Fluorescence- A.model: Maximum fluorescence- integral.model: Integral'

Value

An `flFit` object that contains all fluorescence fitting results, compatible with various plotting functions of the QurvE package.

raw.x	Raw x matrix passed to the function as `time` (for x_type = 'time') or `growth` (for x_type = 'growth').
raw.fl	Raw growth dataframe passed to the function as `data`.
flTable	Table with fluorescence parameters and related statistics for each fluorescence curve evaluation performed by the function. This table, which is also returned by the generic `summary.flFit` method applied to a `flFit` object, is used as an input for `fl.drFit`.
flFittedLinear	List of all `flFitLinear` objects, generated by the call of `flFitLinear`. Note: access to each object in the list via double brace: flFittedLinear[[#n]].
flFittedSplines	List of all `flFitSpline` objects, generated by the call of `flFitSpline`. Note: access to each object via double brace: flFittedSplines[[#n]].
flBootSplines	List of all `flBootSpline` objects, generated by the call of `flBootSpline`. Note: access to each object via double brace: flFittedSplines[[#n]].
control	Object of class `fl.control` containing list of options passed to the function as `control`.

See Also

Other workflows: `growth.gcFit()`, `growth.workflow()`

Other fluorescence fitting functions: `flBootSpline()`, `flFitSpline()`

Other dose-response analysis functions: `growth.drBootSpline()`, `growth.drFitSpline()`, `growth.gcFit()`, `growth.workflow()`

Examples

```
# load example dataset
input <- read_data(data.growth = system.file("lac_promoters_growth.txt", package = "QurvE"),
              data.fl = system.file("lac_promoters_fluorescence.txt", package = "QurvE"),
                   csvsep = "\t",
                   csvsep.fl = "\t" )

# Define fit controls
control <- fl.control(fit.opt = "s",
             x_type = "time", norm_fl = TRUE,
             dr.parameter = "max_slope.spline",
             dr.method = "model",
             suppress.messages = TRUE)

# Run curve fitting workflow
res <- flFit(fl_data = input$norm.fluorescence,
             time = input$time,
             control = control,
             parallelize = FALSE)

summary(res)
```

`flFitLinear` *Data fit via a heuristic linear method*

Description

Determine maximum slopes from using a heuristic approach similar to the "growth rates made easy"-method of Hall et al. (2013).

Usage

```
flFitLinear(
  time = NULL,
  growth = NULL,
  fl_data,
  ID = "undefined",
  quota = 0.95,
 control = fl.control(x_type = c("growth", "time"), log.x.lin = FALSE, log.y.lin =
  FALSE, t0 = 0, min.growth = NA, lin.h = NULL, lin.R2 = 0.98, lin.RSD = 0.05, lin.dY =
    0.05, biphasic = FALSE)
)
```

Arguments

`time`	Vector of the independent time variable (if x_type = "time" in control object).
`growth`	Vector of the independent time growth (if x_type = "growth" in control object).

fl_data	Vector of the dependent fluorescence variable.
ID	(Character) The name of the analyzed sample.
quota	(Numeric, between 0 an 1) Define what fraction of max_slope the slope of regression windows adjacent to the window with highest slope should have to be included in the overall linear fit.
control	A fl.control object created with fl.control, defining relevant fitting options.

Value

A gcFitLinear object with parameters of the fit. The lag time is estimated as the intersection between the fit and the horizontal line with $y = y_0$, where y0 is the first value of the dependent variable. Use plot.gcFitSpline to visualize the linear fit.

raw.x	Filtered x values used for the spline fit.
raw.fl	Filtered fluorescence values used for the spline fit.
filt.x	Filtered x values.
filt.fl	Filtered fluorescence values.
ID	(Character) Identifies the tested sample.
FUN	Linear *function* used for plotting the tangent at mumax.
fit	lm object; result of the final call of lm to perform the linear regression.
par	List of determined fluorescence parameters:

- y0: Minimum fluorescence value considered for the heuristic linear method.
- dY: Difference in maximum fluorescence and minimum fluorescence
- A: Maximum fluorescence
- y0_lm: Intersection of the linear fit with the abscissa.
- max_slope: Maximum slope of the linear fit.
- tD: Doubling time.
- slope.se: Standard error of the maximum slope.
- lag: Lag X.
- x.max_start: X value of the first data point within the window used for the linear regression.
- x.max_end: X value of the last data point within the window used for the linear regression.
- x.turn: For biphasic: X at the inflection point that separates two phases.
- max.slope2: For biphasic: Slope of the second phase.
- tD2: Doubling time of the second phase.
- y0_lm2: For biphasic: Intersection of the linear fit of the second phase with the abscissa.
- lag2: For biphasic: Lag time determined for the second phase..
- x.max2_start: For biphasic: X value of the first data point within the window used for the linear regression of the second phase.
- x.max2_end: For biphasic: X value of the last data point within the window used for the linear regression of the second phase.

ndx	Index of data points used for the linear regression.
ndx2	Index of data points used for the linear regression for the second phase.
control	Object of class grofit.control containing list of options passed to the function as control.
rsquared	R^2 of the linear regression.
rsquared2	R^2 of the linear regression for the second phase.
fitFlag	(Logical) Indicates whether linear regression was successfully performed on the data.
fitFlag2	(Logical) Indicates whether a second phase was identified.
reliable	(Logical) Indicates whether the performed fit is reliable (to be set manually).

References

Hall, BG., Acar, H, Nandipati, A and Barlow, M (2014) Growth Rates Made Easy. Mol. Biol. Evol. 31: 232-38, DOI: 10.1093/molbev/mst187

Petzoldt T (2022). *growthrates: Estimate Growth Rates from Experimental Data*. R package version 0.8.3, https://CRAN.R-project.org/package=growthrates.

Examples

```
# load example dataset
input <- read_data(data.growth = system.file("lac_promoters_growth.txt", package = "QurvE"),
              data.fl = system.file("lac_promoters_fluorescence.txt", package = "QurvE"),
                   csvsep = "\t",
                   csvsep.fl = "\t")

# Extract time and normalized fluorescence data for single sample
time <- input$time[4,]
data <- input$norm.fluorescence[4,-(1:3)] # Remove identifier columns

# Perform linear fit
TestFit <- flFitLinear(time = time,
                       fl_data = data,
                       ID = "TestFit",
                       control = fl.control(fit.opt = "l", x_type = "time",
                       lin.R2 = 0.95, lin.RSD = 0.1,
                       lin.h = 20))

plot(TestFit)
```

---

flFitSpline *Perform a smooth spline fit on fluorescence data*

Description

flFitSpline performs a smooth spline fit on the dataset and determines the greatest slope as the global maximum in the first derivative of the spline.

Usage

```
flFitSpline(
  time = NULL,
  growth = NULL,
  fl_data,
  ID = "undefined",
 control = fl.control(biphasic = FALSE, x_type = c("growth", "time"), log.x.spline =
    FALSE, log.y.spline = FALSE, smooth.fl = 0.75, t0 = 0, min.growth = NA)
)
```

Arguments

time	Vector of the independent variable: time (if x_type = 'time' in fl.control object.
growth	Vector of the independent variable: growth (if x_type = 'growth' in fl.control object.
fl_data	Vector of dependent variable: fluorescence.
ID	(Character) The name of the analyzed sample.
control	A fl.control object created with fl.control, defining relevant fitting options.
biphasic	(Logical) Shall flFitLinear and flFitSpline try to extract fluorescence parameters for two different phases (as observed with, e.g., regulator-promoter systems with varying response in different growth stages) (TRUE) or not (FALSE)?
x_type	(Character) Which data type shall be used as independent variable? Options are 'growth' and 'time'.
log.x.spline	(Logical) Indicates whether *ln(x+1)* should be applied to the independent variable for *spline* fits. Default: FALSE.
log.y.spline	(Logical) Indicates whether *ln(y/y0)* should be applied to the fluorescence data for *spline* fits. Default: FALSE
smooth.fl	(Numeric) Parameter describing the smoothness of the spline fit; usually (not necessary) within (0;1]. smooth.gc=NULL causes the program to query an optimal value via cross validation techniques. Especially for datasets with few data points the option NULL might cause a too small smoothing parameter. This can result a too tight fit that is susceptible to measurement errors (thus overestimating slopes) or produce an error in smooth.spline or lead to overfitting. The usage of a fixed value is recommended for reproducible results across samples. See smooth.spline for further details. Default: 0.55
t0	(Numeric) Minimum time value considered for linear and spline fits.
min.growth	(Numeric) Indicate whether only values above a certain threshold should be considered for linear regressions or spline fits.

Details

If biphasic = TRUE, the following steps are performed to define a second phase:

1. Determine local minima within the first derivative of the smooth spline fit.

2. Remove the 'peak' containing the highest value of the first derivative (i.e., mu_{max}) that is flanked by two local minima.
3. Repeat the smooth spline fit and identification of maximum slope for later time values than the local minimum after mu_{max}.
4. Repeat the smooth spline fit and identification of maximum slope for earlier time values than the local minimum before mu_{max}.
5. Choose the greater of the two independently determined slopes as $mu_{max}2$.

Value

A `flFitSpline` object. The lag time is estimated as the intersection between the tangent at the maximum slope and the horizontal line with $y = y_0$, where `y0` is the first value of the dependent variable. Use `plot.flFitSpline` to visualize the spline fit and derivative over time.

`x.in`	Raw x values provided to the function as `time` or `growth`.
`fl.in`	Raw fluorescence data provided to the function as `fl_data`.
`raw.x`	Filtered x values used for the spline fit.
`raw.fl`	Filtered fluorescence values used for the spline fit.
`ID`	(Character) Identifies the tested sample.
`fit.x`	Fitted x values.
`fit.fl`	Fitted fluorescence values.
`parameters`	List of determined parameters.

- `A`: Maximum fluorescence.
- `dY`: Difference in maximum fluorescence and minimum fluorescence.
- `max_slope`: Maximum slope of fluorescence-vs.-x data (i.e., maximum in first derivative of the spline).
- `x.max`: Time at the maximum slope.
- `lambda`: Lag time.
- `b.tangent`: Intersection of the tangent at the maximum slope with the abscissa.
- `max_slope2`: For biphasic course of fluorescence: Maximum slope of fluorescence-vs.-x data of the second phase.
- `lambda2`: For biphasic course of fluorescence: Lag time determined for the second phase.
- `x.max2`: For biphasic course of fluorescence: Time at the maximum slope of the second phase.
- `b.tangent2`: For biphasic course of fluorescence: Intersection of the tangent at the maximum slope of the second phase with the abscissa.
- `integral`: Area under the curve of the spline fit.

`spline`	`smooth.spline` object generated by the `smooth.spline` function.
`spline.deriv1`	list of time ('x') and growth ('y') values describing the first derivative of the spline fit.
`reliable`	(Logical) Indicates whether the performed fit is reliable (to be set manually).
`fitFlag`	(Logical) Indicates whether a spline fit was successfully performed on the data.
`fitFlag2`	(Logical) Indicates whether a second phase was identified.
`control`	Object of class `fl.control` containing list of options passed to the function as `control`.

See Also

Other fluorescence fitting functions: `flBootSpline()`, `flFit()`

Examples

```
# load example dataset
input <- read_data(data.growth = system.file("lac_promoters_growth.txt", package = "QurvE"),
              data.fl = system.file("lac_promoters_fluorescence.txt", package = "QurvE"),
                   csvsep = "\t",
                   csvsep.fl = "\t")

# Extract time and normalized fluorescence data for single sample
time <- input$time[4,]
data <- input$norm.fluorescence[4,-(1:3)] # Remove identifier columns

# Perform linear fit
TestFit <- flFitSpline(time = time,
                       fl_data = data,
                       ID = 'TestFit',
                       control = fl.control(fit.opt = 's', x_type = 'time'))

plot(TestFit)
```

`growth.control` *Create a* `grofit.control` *object.*

Description

A `grofit.control` object is required to perform various computations on growth data stored within `grodata` objects (created with `read_data` or `parse_data`). A `grofit.control` object is created automatically as part of `growth.workflow`.

Usage

```
growth.control(
  neg.nan.act = FALSE,
  clean.bootstrap = TRUE,
  suppress.messages = FALSE,
  fit.opt = c("a"),
  t0 = 0,
  tmax = NA,
  min.growth = NA,
  max.growth = NA,
  log.x.gc = FALSE,
  log.y.lin = TRUE,
  log.y.spline = TRUE,
  log.y.model = TRUE,
  lin.h = NULL,
```

```
  lin.R2 = 0.97,
  lin.RSD = 0.1,
  lin.dY = 0.05,
  biphasic = FALSE,
  interactive = FALSE,
  nboot.gc = 0,
  smooth.gc = 0.55,
 model.type = c("logistic", "richards", "gompertz", "gompertz.exp", "huang", "baranyi"),
  dr.method = c("model", "spline"),
 dr.model = c("gammadr", "multi2", "LL.2", "LL.3", "LL.4", "LL.5", "W1.2", "W1.3",
   "W1.4", "W2.2", "W2.3", "W2.4", "LL.3u", "LL2.2", "LL2.3", "LL2.3u", "LL2.4",
    "LL2.5", "AR.2", "AR.3", "MM.2"),
  dr.have.atleast = 6,
 dr.parameter = c("mu.linfit", "lambda.linfit", "dY.linfit", "A.linfit", "mu.spline",
   "lambda.spline", "dY.spline", "A.spline", "mu.model", "lambda.model",
   "dY.orig.model", "A.orig.model"),
  smooth.dr = NULL,
  log.x.dr = FALSE,
  log.y.dr = FALSE,
  nboot.dr = 0,
  growth.thresh = 1.5
)
```

Arguments

neg.nan.act	(Logical) Indicates whether the program should stop when negative growth values or NA values appear (TRUE). Otherwise, the program removes these values silently (FALSE). Improper values may be caused by incorrect data or input errors. Default: FALSE.
clean.bootstrap	(Logical) Determines if negative values which occur during bootstrap should be removed (TRUE) or kept (FALSE). Note: Infinite values are always removed. Default: TRUE.
suppress.messages	(Logical) Indicates whether messages (information about current growth curve, EC50 values etc.) should be displayed (FALSE) or not (TRUE). This option is meant to speed up the processing of high throughput data. Note: warnings are still displayed. Default: FALSE.
fit.opt	(Character or character vector) Indicates whether the program should perform a linear regression ('l'), model fit ('m'), spline fit ('s'), or all ('a'). Combinations can be freely chosen by providing a character vector, e.g. fit.opt = c('l', 's') Default: fit.opt = c('l', 's').
t0	(Numeric) Minimum time value considered for linear and spline fits.
tmax	(Numeric) Maximum time value considered for linear and spline fits.
min.growth	(Numeric) Indicate whether only growth values above a certain threshold should be considered for linear regressions or spline fits.
max.growth	(Numeric) Indicate whether only growth values below a certain threshold should be considered for linear regressions or spline fits.

`log.x.gc` (Logical) Indicates whether *ln(x+1)* should be applied to the time data for *linear* and *spline* fits. Default: `FALSE`.

`log.y.lin` (Logical) Indicates whether *ln(y/y0)* should be applied to the growth data for *linear* fits. Default: `TRUE`

`log.y.spline` (Logical) Indicates whether *ln(y/y0)* should be applied to the growth data for *spline* fits. Default: `TRUE`

`log.y.model` (Logical) Indicates whether *ln(y/y0)* should be applied to the growth data for *model* fits. Default: `TRUE`

`lin.h` (Numeric) Manually define the size of the sliding window used in `growth.gcFitLinear` If `NULL`, h is calculated for each samples based on the number of measurements in the growth phase of the plot.

`lin.R2` (Numeric) R^2 threshold for `growth.gcFitLinear`

`lin.RSD` (Numeric) Relative standard deviation (RSD) threshold for the calculated slope in `growth.gcFitLinear`

`lin.dY` (Numeric) Threshold for the minimum fraction of growth increase a linear regression window should cover. Default: 0.05 (5%).

`biphasic` (Logical) Shall `growth.gcFitLinear` and `growth.gcFitSpline` try to extract growth parameters for two different growth phases (as observed with, e.g., diauxic shifts) (`TRUE`) or not (`FALSE`)?

`interactive` (Logical) Controls whether the fit of each growth curve and method is controlled manually by the user. If `TRUE`, each fit is visualized in the *Plots* pane and the user can adjust fitting parameters and confirm the reliability of each fit per sample. Default: `TRUE`.

`nboot.gc` (Numeric) Number of bootstrap samples used for nonparametric growth curve fitting with `growth.gcBootSpline`. Use `nboot.gc = 0` to disable the bootstrap. Default: `0`

`smooth.gc` (Numeric) Parameter describing the smoothness of the spline fit; usually (not necessary) within (0;1]. `smooth.gc=NULL` causes the program to query an optimal value via cross validation techniques. Especially for datasets with few data points the option `NULL` might cause a too small smoothing parameter. This can result a too tight fit that is susceptible to measurement errors (thus overestimating growth rates) or produce an error in `smooth.spline` or lead to overfitting. The usage of a fixed value is recommended for reproducible results across samples. See `smooth.spline` for further details. Default: `0.55`

`model.type` (Character) Vector providing the names of the parametric models which should be fitted to the data. Default: `c('logistic', 'richards', 'gompertz', 'gompertz.exp', 'huang', 'baranyi')`.

`dr.method` (Character) Define the method used to perform a dose-responde analysis: smooth spline fit (`'spline'`) or model fitting (`'model'`).

`dr.model` (Character) Provide a list of models from the R package 'drc' to include in the dose-response analysis (if `dr.method = 'model'`). If more than one model is provided, the best-fitting model will be chosen based on the Akaike Information Criterion.

`dr.have.atleast` (Numeric) Minimum number of different values for the response parameter one should have for estimating a dose response curve. Note: All fit procedures require at least six unique values. Default: `6`.

`dr.parameter` (Character or numeric) The response parameter in the output table to be used for creating a dose response curve. See `growth.drFit` for further details. Default: `'mu.linfit'`, which represents the maximum slope of the linear regression. Typical options include: `'mu.linfit'`, `'lambda.linfit'`, `'dY.linfit'`, `'mu.spline'`, `'dY.spline'`, `'mu.model'`, and `'A.model'`.

`smooth.dr` (Numeric) Smoothing parameter used in the spline fit by smooth.spline during dose response curve estimation. Usually (not necessesary) in (0; 1]. See `smooth.spline` for further details. Default: `NULL`.

`log.x.dr` (Logical) Indicates whether `ln(x+1)` should be applied to the concentration data of the dose response curves. Default: `FALSE`.

`log.y.dr` (Logical) Indicates whether `ln(y+1)` should be applied to the response data of the dose response curves. Default: `FALSE`.

`nboot.dr` (Numeric) Defines the number of bootstrap samples for EC50 estimation. Use `nboot.dr = 0` to disable bootstrapping. Default: `0`.

`growth.thresh` (Numeric) Define a threshold for growth. Only if any growth value in a sample is greater than `growth.thresh` (default: 1.5) times the start growth, further computations are performed. Else, a message is returned.

Value

Generates a list with all arguments described above as entries.

References

Matthias Kahm, Guido Hasenbrink, Hella Lichtenberg-Frate, Jost Ludwig, Maik Kschischo (2010). *grofit: Fitting Biological Growth Curves with R*. Journal of Statistical Software, 33(7), 1-21. DOI: 10.18637/jss.v033.i07

Examples

```
# default option
control_default <- growth.control()
# user defined
control_manual <- growth.control(fit.opt = c('s', 'm'),
                                 smooth.gc = 0.5,
                                 model.type = c('huang', 'baranyi'))
```

`growth.drBootSpline` *Perform a smooth spline fit on response vs. concentration data of a single sample*

Description

`growth.drBootSpline` resamples the values in a dataset with replacement and performs a spline fit for each bootstrap sample to determine the EC50.

Usage

```
growth.drBootSpline(conc, test, drID = "undefined", control = growth.control())
```

Arguments

`conc`	Vector of concentration values.
`test`	Vector of response parameter values of the same length as `conc`.
`drID`	(Character) The name of the analyzed sample.
`control`	A `grofit.control` object created with `growth.control`, defining relevant fitting options.

Value

An object of class `drBootSpline` containing a distribution of growth parameters and a `drFitSpline` object for each bootstrap sample. Use `plot.drBootSpline` to visualize all bootstrapping splines as well as the distribution of EC50.

`raw.conc`	Raw data provided to the function as `conc`.
`raw.test`	Raw data for the response parameter provided to the function as `test`.
`drID`	(Character) Identifies the tested condition.
`boot.conc`	Table of concentration values per column, resulting from each spline fit of the bootstrap.
`boot.test`	Table of response values per column, resulting from each spline fit of the bootstrap.
`boot.drSpline`	List containing all `drFitSpline` objects generated by the call of `growth.drFitSpline`.
`ec50.boot`	Vector of estimated EC50 values from each bootstrap entry.
`ec50y.boot`	Vector of estimated response at EC50 values from each bootstrap entry.
`BootFlag`	(Logical) Indicates the success of the bootstrapping operation.
`control`	Object of class `grofit.control` containing list of options passed to the function as `control`.

References

Matthias Kahm, Guido Hasenbrink, Hella Lichtenberg-Frate, Jost Ludwig, Maik Kschischo (2010). *grofit: Fitting Biological Growth Curves with R*. Journal of Statistical Software, 33(7), 1-21. DOI: 10.18637/jss.v033.i07

See Also

Other dose-response analysis functions: `flFit()`, `growth.drFitSpline()`, `growth.gcFit()`, `growth.workflow()`

Examples

```
conc <- c(0, rev(unlist(lapply(1:18, function(x) 10*(2/3)^x))),10)
response <- c(1/(1+exp(-0.7*(4-conc[-20])))+rnorm(19)/50, 0)

TestRun <- growth.drBootSpline(conc, response, drID = 'test',
               control = growth.control(log.x.dr = TRUE, smooth.dr = 0.8,
                                        nboot.dr = 50))

print(summary(TestRun))
plot(TestRun, combine = TRUE)
```

---

growth.drFit *Perform a dose-response analysis on response vs. concentration data*

Description

`growth.drFit` serves to determine dose-response curves on every condition in a dataset. The response parameter can be chosen from every physiological parameter in a `gcTable` table which is obtained via `growth.gcFit`. `growth.drFit` calls the functions `growth.drFitSpline` and `growth.drBootSpline`, or `growth.drFitModel` to generate a table with estimates for EC50 and respecting statistics.

Usage

```
growth.drFit(
  gcTable,
 control = growth.control(dr.method = "model", dr.model = c("gammadr", "multi2", "LL.2",
  "LL.3", "LL.4", "LL.5", "W1.2", "W1.3", "W1.4", "W2.2", "W2.3", "W2.4", "LL.3u",
    "LL2.2", "LL2.3", "LL2.3u", "LL2.4", "LL2.5", "AR.2", "AR.3", "MM.2"),
  dr.have.atleast = 6, dr.parameter = "mu.linear", nboot.dr = 0, smooth.dr = NULL,
    log.x.dr = FALSE, log.y.dr = FALSE)
)
```

Arguments

`gcTable`	A dataframe containing the data for the dose-response curve estimation. Such table of class `gcTable` can be obtained by running `growth.gcFit`.
`control`	A `grofit.control` object created with `growth.control`, defining relevant fitting options.
`dr.method`	(Character) Define the method used to perform a dose-responde analysis: smooth spline fit (`'spline'`) or model fitting (`'model'`).

`dr.model` (Character) Provide a list of models from the R package 'drc' to include in the dose-response analysis (if `dr.method = 'model'`). If more than one model is provided, the best-fitting model will be chosen based on the Akaike Information Criterion.

`dr.have.atleast` (Numeric) Minimum number of different values for the response parameter one should have for estimating a dose response curve. Note: All fit procedures require at least six unique values. Default: `6`.

`dr.parameter` (Character or numeric) The response parameter in the output table to be used for creating a dose response curve. See `growth.drFit` for further details. Default: `'mu.linfit'`, which represents the maximum slope of the linear regression. Typical options include: `'mu.linfit'`, `'lambda.linfit'`, `'dY.linfit'`, `'mu.spline'`, `'dY.spline'`, `'mu.model'`, and `'A.model'`.

`smooth.dr` (Numeric) Smoothing parameter used in the spline fit by smooth.spline during dose response curve estimation. Usually (not necessesary) in (0; 1]. See `smooth.spline` for further details. Default: `NULL`.

`log.x.dr` (Logical) Indicates whether `ln(x+1)` should be applied to the concentration data of the dose response curves. Default: `FALSE`.

`log.y.dr` (Logical) Indicates whether `ln(y+1)` should be applied to the response data of the dose response curves. Default: `FALSE`.

`nboot.dr` (Numeric) Defines the number of bootstrap samples for EC50 estimation. Use `nboot.dr = 0` to disable bootstrapping. Default: `0`.

Details

Common response parameters used in dose-response analysis:Linear fit:- mu.linfit: Growth rate- lambda.linfit: Lag time- dY.linfit: Density increase- A.linfit: Maximum measurementSpline fit:- mu.spline: Growth rate- lambda.spline: Lag time- A.spline: Maximum measurement- dY.spline: Density increase- integral.spline: IntegralParametric fit:- mu.model: Growth rate- lambda.model: Lag time- A.model: Maximum measurement- integral.model: Integral'

Value

An object of class `drFit`.

`raw.data` Data that passed to the function as `gcTable`.

`drTable` Dataframe containing condition identifiers, fit options, and results of the dose-response analysis.

`drBootSplines` List of all `drBootSpline` objects generated by the call of `growth.drBootSpline` for each distinct experiment.

`drFittedSplines` List of all `drFitSpline` objects generated by the call of `growth.drFitSpline` for each distinct experiment.

`control` Object of class `grofit.control` containing list of options passed to the function as `control`.

References

Matthias Kahm, Guido Hasenbrink, Hella Lichtenberg-Frate, Jost Ludwig, Maik Kschischo (2010). *grofit: Fitting Biological Growth Curves with R*. Journal of Statistical Software, 33(7), 1-21. DOI: 10.18637/jss.v033.i07

See Also

Other growth fitting functions: `growth.gcBootSpline()`, `growth.gcFitLinear()`, `growth.gcFitModel()`, `growth.gcFitSpline()`, `growth.gcFit()`, `growth.workflow()`

Examples

```
# Create random growth data set
rnd.data1 <- rdm.data(d = 35, mu = 0.8, A = 5, label = 'Test1')
rnd.data2 <- rdm.data(d = 35, mu = 0.6, A = 4.5, label = 'Test2')

rnd.data <- list()
rnd.data[['time']] <- rbind(rnd.data1$time, rnd.data2$time)
rnd.data[['data']] <- rbind(rnd.data1$data, rnd.data2$data)

# Run growth curve analysis workflow
gcFit <- growth.gcFit(time = rnd.data$time,
                      data = rnd.data$data,
                      parallelize = FALSE,
                      control = growth.control(fit.opt = 's',
                                               suppress.messages = TRUE))

# Perform dose-response analysis
drFit <- growth.drFit(gcTable = gcFit$gcTable,
            control = growth.control(dr.parameter = 'mu.spline'))

# Inspect results
summary(drFit)
plot(drFit)
```

---

growth.drFitModel *Fit various models to response vs. concentration data of a single sample to determine the EC50.*

Description

Fit various models to response vs. concentration data of a single sample to determine the EC50.

Usage

```
growth.drFitModel(conc, test, drID = "undefined", control = growth.control())
```

Arguments

conc	Vector of concentration values.
test	Vector of response parameter values of the same length as conc.
drID	(Character) The name of the analyzed condition
control	A grofit.control object created with growth.control, defining relevant fitting options.

Value

A drFitModel object.

References

Christian Ritz, Florent Baty, Jens C. Streibig, Daniel Gerhard (2015). *Dose-Response Analysis Using R*. PLoS ONE 10(12): e0146021. DOI: 10.1371/journal.pone.0146021

Examples

```
conc <- c(0, rev(unlist(lapply(1:18, function(x) 10*(2/3)^x))),10)
response <- c(1/(1+exp(-0.7*(4-conc[-20])))+rnorm(19)/50, 0)

TestRun <- growth.drFitModel(conc, response, drID = 'test')

print(summary(TestRun))
plot(TestRun)
```

---

growth.drFitSpline *Perform a smooth spline fit on response vs. concentration data of a single sample to determine the EC50.*

Description

growth.drFitSpline performs a smooth spline fit determines the EC50 as the concentration at the half-maximum value of the response parameter of the spline.

Usage

```
growth.drFitSpline(conc, test, drID = "undefined", control = growth.control())
```

Arguments

conc	Vector of concentration values.
test	Vector of response parameter values of the same length as conc.
drID	(Character) The name of the analyzed condition
control	A grofit.control object created with growth.control, defining relevant fitting options.

Details

During the spline fit with smooth.spline, higher weights are assigned to data points with a concentration value of 0, as well as to x-y pairs with a response parameter value of 0 and pairs at concentration values before zero-response parameter values.

Value

A drFitSpline object.

raw.conc	Raw data provided to the function as conc.
raw.test	Raw data for the response parameter provided to the function as test.
drID	(Character) Identifies the tested condition
fit.conc	Fitted concentration values.
fit.test	Fitted response values.
spline	smooth.spline object generated by the smooth.spline function.
spline.low	x and y values of lowess spline fit on raw data. Used to call smooth.spline.
parameters	List of parameters estimated from dose response curve fit.

- EC50: Concentration at half-maximal response.
- yEC50: Response value related to EC50.
- EC50.orig: EC50 value in original scale, if a transformation was applied.
- yEC50.orig: Response value for EC50 in original scale, if a transformation was applied.

fitFlag	(Logical) Indicates whether a spline could fitted successfully to data.
reliable	(Logical) Indicates whether the performed fit is reliable (to be set manually).
control	Object of class grofit.control containing list of options passed to the function as control.

Use plot.drFitSpline to visualize the spline fit.

References

Matthias Kahm, Guido Hasenbrink, Hella Lichtenberg-Frate, Jost Ludwig, Maik Kschischo (2010). *grofit: Fitting Biological Growth Curves with R*. Journal of Statistical Software, 33(7), 1-21. DOI: 10.18637/jss.v033.i07

Christian Ritz, Florent Baty, Jens C. Streibig, Daniel Gerhard (2015). *Dose-Response Analysis Using R*. PLoS ONE 10(12): e0146021. DOI: 10.1371/journal.pone.0146021

See Also

Other dose-response analysis functions: flFit(), growth.drBootSpline(), growth.gcFit(), growth.workflow()

Examples

```
conc <- c(0, rev(unlist(lapply(1:18, function(x) 10*(2/3)^x))),10)
response <- c(1/(1+exp(-0.7*(4-conc[-20])))+rnorm(19)/50, 0)

TestRun <- growth.drFitSpline(conc, response, drID = 'test',
             control = growth.control(log.x.dr = TRUE, smooth.dr = 0.8))

print(summary(TestRun))

plot(TestRun)
```

---

growth.gcBootSpline *Perform a bootstrap on growth vs. time data followed by spline fits for each resample*

Description

`growth.gcBootSpline` resamples the growth-time value pairs in a dataset with replacement and performs a spline fit for each bootstrap sample.

Usage

```
growth.gcBootSpline(time, data, gcID = "undefined", control = growth.control())
```

Arguments

`time`	Vector of the independent variable (usually: time).
`data`	Vector of dependent variable (usually: growth values).
`gcID`	(Character) The name of the analyzed sample.
`control`	A `grofit.control` object created with `growth.control`, defining relevant fitting options.

Value

A `gcBootSpline` object containing a distribution of growth parameters and a `gcFitSpline` object for each bootstrap sample. Use `plot.gcBootSpline` to visualize all bootstrapping splines as well as the distribution of physiological parameters.

`raw.time`	Raw time values provided to the function as `time`.
`raw.data`	Raw growth data provided to the function as `data`.
`gcID`	(Character) Identifies the tested sample.
`boot.time`	Table of time values per column, resulting from each spline fit of the bootstrap.
`boot.data`	Table of growth values per column, resulting from each spline fit of the bootstrap.
`boot.gcSpline`	List of `gcFitSpline` object, created by `growth.gcFitSpline` for each resample of the bootstrap.

lambda	Vector of estimated lambda (lag time) values from each bootstrap entry.
mu	Vector of estimated mu (maximum growth rate) values from each bootstrap entry.
A	Vector of estimated A (maximum growth) values from each bootstrap entry.
integral	Vector of estimated integral values from each bootstrap entry.
bootFlag	(Logical) Indicates the success of the bootstrapping operation.
control	Object of class grofit.control containing list of options passed to the function as control.

References

Matthias Kahm, Guido Hasenbrink, Hella Lichtenberg-Frate, Jost Ludwig, Maik Kschischo (2010). *grofit: Fitting Biological Growth Curves with R*. Journal of Statistical Software, 33(7), 1-21. DOI: 10.18637/jss.v033.i07

See Also

Other growth fitting functions: growth.drFit(), growth.gcFitLinear(), growth.gcFitModel(), growth.gcFitSpline(), growth.gcFit(), growth.workflow()

Examples

```
# Create random growth dataset
rnd.dataset <- rdm.data(d = 35, mu = 0.8, A = 5, label = 'Test1')

# Extract time and growth data for single sample
time <- rnd.dataset$time[1,]
data <- rnd.dataset$data[1,-(1:3)] # Remove identifier columns

# Introduce some noise into the measurements
data <- data + stats::runif(97, -0.01, 0.09)

# Perform bootstrapping spline fit
TestFit <- growth.gcBootSpline(time, data, gcID = 'TestFit',
              control = growth.control(fit.opt = 's', nboot.gc = 50))

plot(TestFit, combine = TRUE, lwd = 0.5)
```

---

growth.gcFit — *Perform a growth curve analysis on all samples in the provided dataset.*

Description

growth.gcFit performs all computational growth fitting operations based on the user input.

Usage

```
growth.gcFit(time, data, control = growth.control(), parallelize = TRUE, ...)
```

Arguments

time	(optional) A matrix containing time values for each sample.
data	Either... 1. a grodata object created with read_data or parse_data, 2. a list containing a 'time' matrix as well as 'growth' and, if appropriate, a 'fluorescence' dataframes, or 3. a dataframe containing growth values (if a time matrix is provided as separate argument).
control	A grofit.control object created with growth.control, defining relevant fitting options.
parallelize	Run linear fits and bootstrapping operations in parallel using all but one available processor cores
...	Further arguments passed to the shiny app.

Value

A gcFit object that contains all growth fitting results, compatible with various plotting functions of the QurvE package.

raw.time	Raw time matrix passed to the function as time.
raw.data	Raw growth dataframe passed to the function as data.
gcTable	Table with growth parameters and related statistics for each growth curve evaluation performed by the function. This table, which is also returned by the generic summary.gcFit method applied to a gcFit object, is used as an input for growth.drFit.
gcFittedLinear	List of all gcFitLinear objects, generated by the call of growth.gcFitLinear. Note: access to each object in the list via double brace: gcFittedLinear[[#n]].
gcFittedModels	List of all gcFitModel objects, generated by the call of growth.gcFitModel. Note: access to each object in the list via double brace: gcFittedModels[[#n]].
gcFittedSplines	List of all gcFitSpline objects, generated by the call of growth.gcFitSpline. Note: access to each object via double brace: gcFittedSplines[[#n]].
gcBootSplines	List of all gcBootSpline objects, generated by the call of growth.gcBootSpline. Note: access to each object via double brace: gcFittedSplines[[#n]].
control	Object of class grofit.control containing list of options passed to the function as control.

References

Matthias Kahm, Guido Hasenbrink, Hella Lichtenberg-Frate, Jost Ludwig, Maik Kschischo (2010). *grofit: Fitting Biological Growth Curves with R*. Journal of Statistical Software, 33(7), 1-21. DOI: 10.18637/jss.v033.i07

See Also

Other workflows: flFit(), growth.workflow()

Other growth fitting functions: growth.drFit(), growth.gcBootSpline(), growth.gcFitLinear(), growth.gcFitModel(), growth.gcFitSpline(), growth.workflow()

Other dose-response analysis functions: flFit(), growth.drBootSpline(), growth.drFitSpline(), growth.workflow()

Examples

```
# Create random growth data set
  rnd.data1 <- rdm.data(d = 35, mu = 0.8, A = 5, label = 'Test1')
  rnd.data2 <- rdm.data(d = 35, mu = 0.6, A = 4.5, label = 'Test2')

  rnd.data <- list()
  rnd.data[['time']] <- rbind(rnd.data1$time, rnd.data2$time)
  rnd.data[['data']] <- rbind(rnd.data1$data, rnd.data2$data)

# Run growth curve analysis workflow
  res <- growth.gcFit(time = rnd.data$time,
                      data = rnd.data$data,
                      parallelize = FALSE,
                      control = growth.control(suppress.messages = TRUE,
                                               fit.opt = 's'))
```

---

growth.gcFitLinear *Fit an exponential growth model with a heuristic linear method*

Description

Determine maximum growth rates from the log-linear part of a growth curve using a heuristic approach similar to the "growth rates made easy"-method of Hall et al. (2013).

Usage

```
growth.gcFitLinear(
  time,
  data,
  gcID = "undefined",
  quota = 0.95,
  control = growth.control(t0 = 0, tmax = NA, log.x.gc = FALSE, log.y.lin = TRUE,
   min.growth = NA, max.growth = NA, lin.h = NULL, lin.R2 = 0.97, lin.RSD = 0.1, lin.dY
    = 0.05, biphasic = FALSE)
)
```

Arguments

time	Vector of the independent variable (usually: time).
data	Vector of dependent variable (usually: growth values).
gcID	(Character) The name of the analyzed sample.
quota	(Numeric, between 0 an 1) Define what fraction of mu_{max} the slope of regression windows adjacent to the window with highest slope should have to be included in the overall linear fit.
control	A grofit.control object created with growth.control, defining relevant fitting options.
log.x.gc	(Logical) Indicates whether *ln(x+1)* should be applied to the time data for *linear* and *spline* fits. Default: FALSE.
log.y.lin	(Logical) Indicates whether *ln(y/y0)* should be applied to the growth data for *linear* fits. Default: TRUE
min.growth	(Numeric) Indicate whether only growth values above a certain threshold should be considered for linear regressions.
max.growth	(Numeric) Indicate whether only growth values below a certain threshold should be considered for linear regressions.
t0	(Numeric) Minimum time value considered for linear and spline fits.
tmax	(Numeric) Minimum time value considered for linear and spline fits.
lin.h	(Numeric) Manually define the size of the sliding window . If NULL, h is calculated for each samples based on the number of measurements in the growth phase of the plot.
lin.R2	(Numeric) R^2 threshold for growth.gcFitLinear
lin.RSD	(Numeric) Relative standard deviation (RSD) threshold for calculated slope in growth.gcFitLinear
lin.dY	(Numeric) Enter the minimum percentage of growth increase that a linear regression should cover.
biphasic	(Logical) Shall growth.gcFitLinear try to extract growth parameters for two different growth phases (as observed with, e.g., diauxic shifts) (TRUE) or not (FALSE)?

Details

The algorithm works as follows:

1. Fit linear regressions (Theil-Sen estimator) to all subsets of h consecutive, log-transformed data points (sliding window of size h). If for example $h = 5$, fit a linear regression to points 1 ... 5, 2 ... 6, 3 ... 7 and so on.
2. Find the subset with the highest slope mu_{max}. Do the R^2 and relative standard deviation (RSD) values of the regression meet the in lin.R2 and lin.RSD defined thresholds and do the data points within the regression window account for a fraction of at least lin.dY of the total growth increase? If not, evaluate the subset with the second highest slope, and so on.
3. Include also the data points of adjacent subsets that have a slope of at least $quota \cdot mumax$, e.g., all regression windows that have at least 95% of the maximum slope.

4. Fit a new linear model to the extended data window identified in step 3.

If `biphasic = TRUE`, the following steps are performed to define a second growth phase:

1. Perform a smooth spline fit on the data with a smoothing factor of 0.5.
2. Calculate the second derivative of the spline fit and perform a smooth spline fit of the derivative with a smoothing factor of 0.4.
3. Determine local maxima and minima in the second derivative.
4. Find the local minimum following mu_{max} and repeat the heuristic linear method for later time values.
5. Find the local maximum before mu_{max} and repeat the heuristic linear method for earlier time values.
6. Choose the greater of the two independently determined slopes as $mu_{max}2$.

Value

A `gcFitLinear` object with parameters of the fit. The lag time is estimated as the intersection between the fit and the horizontal line with $y = y_0$, where `y0` is the first value of the dependent variable. Use `plot.gcFitSpline` to visualize the linear fit.

`raw.time`	Raw time values provided to the function as `time`.
`raw.data`	Raw growth data provided to the function as `data`.
`filt.time`	Filtered time values used for the heuristic linear method.
`filt.data`	Filtered growth values.
`log.data`	Log-transformed, filtered growth values used for the heuristic linear method.
`gcID`	(Character) Identifies the tested sample.
`FUN`	Linear *function* used for plotting the tangent at mumax.
`fit`	`lm` object; result of the final call of `lm` to perform the linear regression.
`par`	List of determined growth parameters:

- `y0`: Minimum growth value considered for the heuristic linear method.
- `dY`: Difference in maximum growth and minimum growth.
- `A`: Maximum growth.
- `y0_lm`: Intersection of the linear fit with the abscissa.
- `mumax`: Maximum growth rate (i.e., slope of the linear fit).
- `tD`: Doubling time.
- `mu.se`: Standard error of the maximum growth rate.
- `lag`: Lag time.
- `tmax_start`: Time value of the first data point within the window used for the linear regression.
- `tmax_end`: Time value of the last data point within the window used for the linear regression.
- `t_turn`: For biphasic growth: Time of the inflection point that separates two growth phases.
- `mumax2`: For biphasic growth: Growth rate of the second growth phase.

- `tD2`: Doubling time of the second growth phase.
- `y0_lm2`: For biphasic growth: Intersection of the linear fit of the second growth phase with the abscissa.
- `lag2`: For biphasic growth: Lag time determined for the second growth phase..
- `tmax2_start`: For biphasic growth: Time value of the first data point within the window used for the linear regression of the second growth phase.
- `tmax2_end`: For biphasic growth: Time value of the last data point within the window used for the linear regression of the second growth phase.

`ndx`	Index of data points used for the linear regression.
`ndx2`	Index of data points used for the linear regression for the second growth phase.
`control`	Object of class `grofit.control` containing list of options passed to the function as `control`.
`rsquared`	R^2 of the linear regression.
`rsquared2`	R^2 of the linear regression for the second growth phase.
`fitFlag`	(Logical) Indicates whether linear regression was successfully performed on the data.
`fitFlag2`	(Logical) Indicates whether a second growth phase was identified.
`reliable`	(Logical) Indicates whether the performed fit is reliable (to be set manually).

References

Hall, BG., Acar, H, Nandipati, A and Barlow, M (2014) Growth Rates Made Easy. *Mol. Biol. Evol.* 31: 232-38, DOI: 10.1093/molbev/mst187

Petzoldt T (2022). growthrates: Estimate Growth Rates from Experimental Data. R package version 0.8.3, https://CRAN.R-project.org/package=growthrates.

Theil, H.(1992). A rank-invariant method of linear and polynomial regression analysis. In: Henri Theil's contributions to economics and econometrics. Springer, pp. 345–381. DOI: 10.1007/978-94-011-2546-8_20

See Also

Other growth fitting functions: `growth.drFit()`, `growth.gcBootSpline()`, `growth.gcFitModel()`, `growth.gcFitSpline()`, `growth.gcFit()`, `growth.workflow()`

Examples

```
# Create random growth dataset
rnd.dataset <- rdm.data(d = 35, mu = 0.8, A = 5, label = "Test1")

# Extract time and growth data for single sample
time <- rnd.dataset$time[1,]
data <- rnd.dataset$data[1,-(1:3)] # Remove identifier columns

# Perform linear fit
TestFit <- growth.gcFitLinear(time, data, gcID = "TestFit",
```

```
                control = growth.control(fit.opt = "l"))

plot(TestFit)
```

`growth.gcFitModel` *Fit nonlinear growth models to growth data*

Description

`growth.gcFitModel` determines a parametric growth model that best describes the data.

Usage

```
growth.gcFitModel(time, data, gcID = "undefined", control = growth.control())
```

Arguments

`time`	Vector of the independent variable (usually time).
`data`	Vector of dependent variable (usually growth values).
`gcID`	(Character) The name of the analyzed sample.
`control`	A `grofit.control` object created with `growth.control`, defining relevant fitting options.

Value

A `gcFitModel` object that contains physiological parameters and information about the best fit. Use `plot.gcFitModel` to visualize the parametric fit and growth equation.

`raw.time`	Raw time values provided to the function as `time`.
`raw.data`	Raw growth data provided to the function as `data`.
`gcID`	(Character) Identifies the tested sample.
`fit.time`	Fitted time values.
`fit.data`	Fitted growth values.
`parameters`	List of determined growth parameters.

- `A`: Maximum growth.
- `dY`: Difference in maximum growth and minimum growth of the fitted model.
- `mu`: Maximum growth rate (i.e., maximum in first derivative of the spline).
- `lambda`: Lag time.
- `b.tangent`: Intersection of the tangent at the maximum growth rate with the abscissa.
- `fitpar`: For some models: list of additional parameters used in the equations describing the growth curve.
- `integral`: Area under the curve of the parametric fit.

model	(Character) The model that obtained the fit with the lowest AIC, determined by AIC.
nls	nls object for the chosen model generated by the nls function.
reliable	(Logical) Indicates whether the performed fit is reliable (to be set manually).
fitFlag	(Logical) Indicates whether a parametric model was successfully fitted on the data.
control	Object of class grofit.control containing list of options passed to the function as control.

References

Matthias Kahm, Guido Hasenbrink, Hella Lichtenberg-Frate, Jost Ludwig, Maik Kschischo (2010). *grofit: Fitting Biological Growth Curves with R*. Journal of Statistical Software, 33(7), 1-21. DOI: 10.18637/jss.v033.i07

See Also

Other growth fitting functions: growth.drFit(), growth.gcBootSpline(), growth.gcFitLinear(), growth.gcFitSpline(), growth.gcFit(), growth.workflow()

Examples

```
# Create random growth dataset
rnd.dataset <- rdm.data(d = 35, mu = 0.8, A = 5, label = 'Test1')

# Extract time and growth data for single sample
time <- rnd.dataset$time[1,]
data <- rnd.dataset$data[1,-(1:3)] # Remove identifier columns

# Perform parametric fit
TestFit <- growth.gcFitModel(time, data, gcID = 'TestFit',
                 control = growth.control(fit.opt = 'm'))

plot(TestFit, basesize = 18, eq.size = 1.5)
```

---

growth.gcFitSpline *Perform a smooth spline fit on growth data*

Description

growth.gcFitSpline performs a smooth spline fit on the dataset and determines the highest growth rate as the global maximum in the first derivative of the spline.

Usage

```
growth.gcFitSpline(
  time,
  data,
  gcID = "undefined",
  control = growth.control(biphasic = FALSE)
)
```

Arguments

time	Vector of the independent variable (usually time).
data	Vector of dependent variable (usually: growth values).
gcID	(Character) The name of the analyzed sample.
control	A grofit.control object created with growth.control, defining relevant fitting options.
biphasic	(Logical) Shall growth.gcFitSpline try to extract growth parameters for two different growth phases (as observed with, e.g., diauxic shifts) (TRUE) or not (FALSE)?

Details

If biphasic = TRUE, the following steps are performed to define a second growth phase:

1. Determine local minima within the first derivative of the smooth spline fit.
2. Remove the 'peak' containing the highest value of the first derivative (i.e., mu_{max}) that is flanked by two local minima.
3. Repeat the smooth spline fit and identification of maximum slope for later time values than the local minimum after mu_{max}.
4. Repeat the smooth spline fit and identification of maximum slope for earlier time values than the local minimum before mu_{max}.
5. Choose the greater of the two independently determined slopes as $mu_{max}2$.

Value

A gcFitSpline object. The lag time is estimated as the intersection between the tangent at the maximum slope and the horizontal line with $y = y_0$, where y0 is the first value of the dependent variable. Use plot.gcFitSpline to visualize the spline fit and derivative over time.

time.in	Raw time values provided to the function as time.
data.in	Raw growth data provided to the function as data.
raw.time	Filtered time values used for the spline fit.
raw.data	Filtered growth values used for the spline fit.
gcID	(Character) Identifies the tested sample.
fit.time	Fitted time values.
fit.data	Fitted growth values.

`parameters` List of determined growth parameters.

- `A`: Maximum growth.
- `dY`: Difference in maximum growth and minimum growth.
- `mu`: Maximum growth rate (i.e., maximum in first derivative of the spline).
- `tD`: Doubling time.
- `t.max`: Time at the maximum growth rate.
- `lambda`: Lag time.
- `b.tangent`: Intersection of the tangent at the maximum growth rate with the abscissa.
- `mu2`: For biphasic growth: Growth rate of the second growth phase.
- `tD2`: Doubling time of the second growth phase.
- `lambda2`: For biphasic growth: Lag time determined for the second growth phase.
- `t.max2`: For biphasic growth: Time at the maximum growth rate of the second growth phase.
- `b.tangent2`: For biphasic growth: Intersection of the tangent at the maximum growth rate of the second growth phase with the abscissa.
- `integral`: Area under the curve of the spline fit.

`spline`	`smooth.spline` object generated by the `smooth.spline` function.
`spline.deriv1`	list of time ('x') and growth ('y') values describing the first derivative of the spline fit.
`reliable`	(Logical) Indicates whether the performed fit is reliable (to be set manually).
`fitFlag`	(Logical) Indicates whether a spline fit was successfully performed on the data.
`fitFlag2`	(Logical) Indicates whether a second growth phase was identified.
`control`	Object of class `grofit.control` containing list of options passed to the function as `control`.

References

Matthias Kahm, Guido Hasenbrink, Hella Lichtenberg-Frate, Jost Ludwig, Maik Kschischo (2010). *grofit: Fitting Biological Growth Curves with R*. Journal of Statistical Software, 33(7), 1-21. DOI: 10.18637/jss.v033.i07

See Also

Other growth fitting functions: `growth.drFit()`, `growth.gcBootSpline()`, `growth.gcFitLinear()`, `growth.gcFitModel()`, `growth.gcFit()`, `growth.workflow()`

Examples

```
# Create random growth dataset
rnd.dataset <- rdm.data(d = 35, mu = 0.8, A = 5, label = 'Test1')

# Extract time and growth data for single sample
time <- rnd.dataset$time[1,]
data <- rnd.dataset$data[1,-(1:3)] # Remove identifier columns
```

```
# Perform spline fit
TestFit <- growth.gcFitSpline(time, data, gcID = 'TestFit',
                 control = growth.control(fit.opt = 's'))

plot(TestFit)
```

`growth.report` *Create a PDF and HTML report with results from a growth curve analysis workflow*

Description

`growth.report` requires a `grofit` object and creates a report in PDF and HTML format that summarizes all results.

Usage

```
growth.report(
  grofit,
  out.dir = tempdir(),
  out.nm = NULL,
  ec50 = FALSE,
  format = c("pdf", "html"),
  export = FALSE,
  parallelize = TRUE,
  ...
)
```

Arguments

`grofit`	A `grofit` object created with `growth.workflow`.
`out.dir`	(Character) The path or name of the folder in which the report files are created. If `NULL`, the folder will be named with a combination of 'Report.growth_' and the current date and time.
`out.nm`	Character or `NULL` Define the name of the report files. If `NULL`, the files will be named with a combination of 'GrowthReport_' and the current date and time.
`ec50`	(Logical) Display results of dose-response analysis (`TRUE`) or not (`FALSE`).
`format`	(Character) Define the file format for the report, PDF (`'pdf'`) and/or HTML (`'html'`). Default: (`c('pdf', 'html')`)
`export`	(Logical) Shall all plots generated in the report be exported as individual PDF and PNG files `TRUE` or not `FALSE`?
`parallelize`	(Logical) Create plots using all but one available processor cores (`TRUE`) or only a single core (`FALSE`).

... Further arguments passed to create a report. Currently supported:

- `mean.grp`: Define groups to combine into common plots in the report based on sample identifiers. Partial matches with sample/group names are accepted. Can be `'all'`, a string vector, or a list of string vectors. Note: The maximum number of sample groups (with unique condition/concentration indicators) is 50. If you have more than 50 groups, option `'all'` will produce the error `! Insufficient values in manual scale. [Number] needed but only 50 provided.`
- `mean.conc`: Define concentrations to combine into common plots in the report. Can be a numeric vector, or a list of numeric vectors.

Details

The template .Rmd file used within this function can be found within the QurvE package installation directory.

Value

`NULL`

Examples

```
## Not run:
# Create random growth data set
  rnd.data <- rdm.data(d = 35, mu = 0.8, A = 5, label = 'Test1')


  # Run growth curve analysis workflow
  res <- growth.workflow(time = rnd.data$time,
                         data = rnd.data$data,
                         fit.opt = 's',
                         ec50 = FALSE,
                         export.res = FALSE,
                         suppress.messages = TRUE,
                         parallelize = FALSE)

  growth.report(res, out.dir = tempdir(), parallelize = FALSE)

## End(Not run)
```

---

growth.workflow *Run a complete growth curve analysis and dose-reponse analysis workflow.*

Description

`growth.workflow` runs `growth.control` to create a `grofit.control` object and then performs all computational fitting operations based on the user input. Finally, if desired, a final report is created in PDF or HTML format that summarizes all results obtained.

Usage

```
growth.workflow(
  grodata = NULL,
  time = NULL,
  data = NULL,
  ec50 = TRUE,
  mean.grp = NA,
  mean.conc = NA,
  neg.nan.act = FALSE,
  clean.bootstrap = TRUE,
  suppress.messages = FALSE,
  fit.opt = c("a"),
  t0 = 0,
  tmax = NA,
  min.growth = NA,
  max.growth = NA,
  log.x.gc = FALSE,
  log.y.lin = TRUE,
  log.y.spline = TRUE,
  log.y.model = TRUE,
  biphasic = FALSE,
  lin.h = NULL,
  lin.R2 = 0.97,
  lin.RSD = 0.1,
  lin.dY = 0.05,
  interactive = FALSE,
  nboot.gc = 0,
  smooth.gc = 0.55,
  model.type = c("logistic", "richards", "gompertz", "gompertz.exp", "huang", "baranyi"),
  dr.method = c("model", "spline"),
  dr.model = c("gammadr", "multi2", "LL.2", "LL.3", "LL.4", "LL.5", "W1.2", "W1.3",
    "W1.4", "W2.2", "W2.3", "W2.4", "LL.3u", "LL2.2", "LL2.3", "LL2.3u", "LL2.4",
    "LL2.5", "AR.2", "AR.3", "MM.2"),
  growth.thresh = 1.5,
  dr.have.atleast = 6,
  dr.parameter = c("mu.linfit", "lambda.linfit", "dY.linfit", "A.linfit", "mu.spline",
    "lambda.spline", "dY.spline", "A.spline", "mu.model", "lambda.model",
    "dY.orig.model", "A.orig.model"),
  smooth.dr = 0.1,
  log.x.dr = FALSE,
  log.y.dr = FALSE,
  nboot.dr = 0,
  report = NULL,
  out.dir = NULL,
  out.nm = NULL,
  export.fig = FALSE,
  export.res = FALSE,
  parallelize = TRUE,
```

```
  ...
)
```

Arguments

grodata	A grodata object created with read_data or parse_data, or a list containing a 'time' matrix as well as a 'growth' dataframe.
time	(optional) A matrix containing time values for each sample.
data	(optional) A dataframe containing growth data (if a time matrix is provided as separate argument).
ec50	(Logical) Perform dose-response analysis (TRUE) or not (FALSE).
mean.grp	('all', a string vector, or a list of string vectors) Define groups to combine into common plots in the final report based on sample identifiers (if report == TRUE). Partial matches with sample/group names are accepted. Note: The maximum number of sample groups (with unique condition/concentration indicators) is 50. If you have more than 50 groups, option 'all' will produce the error ! Insufficient values in manual scale. [Number] needed but only 50 provided.
mean.conc	(A numeric vector, or a list of numeric vectors) Define concentrations to combine into common plots in the final report (if report == TRUE).
neg.nan.act	(Logical) Indicates whether the program should stop when negative growth values or NA values appear (TRUE). Otherwise, the program removes these values silently (FALSE). Improper values may be caused by incorrect data or input errors. Default: FALSE.
clean.bootstrap	(Logical) Determines if negative values which occur during bootstrap should be removed (TRUE) or kept (FALSE). Note: Infinite values are always removed. Default: TRUE.
suppress.messages	(Logical) Indicates whether grofit messages (information about current growth curve, EC50 values etc.) should be displayed (FALSE) or not (TRUE). This option is meant to speed up the high-throughput processing data. Note: warnings are still displayed. Default: FALSE.
fit.opt	(Character or character vector) Indicates whether the program should perform a linear regression ('l'), model fit ('m'), spline fit ('s'), or all ('a'). Combinations can be freely chosen by providing a character vector, e.g. fit.opt = c('l', 's') Default: fit.opt = c('l', 's').
t0	(Numeric) Minimum time value considered for linear and spline fits.
tmax	(Numeric) Maximum time value considered for linear and spline fits.
min.growth	(Numeric) Indicate whether only growth values above a certain threshold should be considered for linear regressions or spline fits.
max.growth	(Numeric) Indicate whether only growth values below a certain threshold should be considered for linear regressions or spline fits.
log.x.gc	(Logical) Indicates whether *ln(x+1)* should be applied to the time data for *linear* and *spline* fits. Default: FALSE.

`log.y.lin` (Logical) Indicates whether *ln(y/y0)* should be applied to the growth data for *linear* fits. Default: `TRUE`

`log.y.spline` (Logical) Indicates whether *ln(y/y0)* should be applied to the growth data for *spline* fits. Default: `TRUE`

`log.y.model` (Logical) Indicates whether *ln(y/y0)* should be applied to the growth data for *model* fits. Default: `TRUE`

`biphasic` (Logical) Shall `growth.gcFitLinear` and `growth.gcFitSpline` try to extract growth parameters for two different growth phases (as observed with, e.g., diauxic shifts) (`TRUE`) or not (`FALSE`)?

`lin.h` (Numeric) Manually define the size of the sliding window used in `growth.gcFitLinear` If `NULL`, h is calculated for each samples based on the number of measurements in the growth phase of the plot.

`lin.R2` (Numeric) R^2 threshold for `growth.gcFitLinear`

`lin.RSD` (Numeric) Relative standard deviation (RSD) threshold for calculated slope in `growth.gcFitLinear`

`lin.dY` (Numeric) Threshold for the minimum fraction of growth increase a linear regression window should cover. Default: 0.05 (5%).

`interactive` (Logical) Controls whether the fit of each growth curve and method is controlled manually by the user. If `TRUE`, each fit is visualized in the *Plots* pane and the user can adjust fitting parameters and confirm the reliability of each fit per sample. Default: `TRUE`.

`nboot.gc` (Numeric) Number of bootstrap samples used for nonparametric growth curve fitting with `growth.gcBootSpline`. Use `nboot.gc = 0` to disable the bootstrap. Default: `0`

`smooth.gc` (Numeric) Parameter describing the smoothness of the spline fit; usually (not necessary) within (0;1]. `smooth.gc=NULL` causes the program to query an optimal value via cross validation techniques. Especially for datasets with few data points the option NULL might cause a too small smoothing parameter. This can result a too tight fit that is susceptible to measurement errors (thus overestimating growth rates) or produce an error in `smooth.spline` or lead to an overestimation. The usage of a fixed value is recommended for reproducible results across samples. See `?smooth.spline` for further details. Default: `0.55`

`model.type` (Character) Vector providing the names of the parametric models which should be fitted to the data. Default: `c('logistic', 'richards', 'gompertz', 'gompertz.exp', 'huang', 'baranyi')`.

`dr.method` (Character) Define the method used to perform a dose-responde analysis: smooth spline fit (`'spline'`) or model fitting (`'model'`).

`dr.model` (Character) Provide a list of models from the R package 'drc' to include in the dose-response analysis (if `dr.method = 'model'`). If more than one model is provided, the best-fitting model will be chosen based on the Akaike Information Criterion.

`growth.thresh` (Numeric) Define a threshold for growth. Only if any growth value in a sample is greater than `growth.thresh` (default: 1.5) times the start growth, further computations are performed. Else, a message is returned.

`dr.have.atleast`
: (Numeric) Minimum number of different values for the response parameter one should have for estimating a dose response curve. Note: All fit procedures require at least six unique values. Default: `6`.

`dr.parameter`
: (Character or numeric) The response parameter in the output table to be used for creating a dose response curve. See `growth.drFit` for further details. Default: `'mu.linfit'`, which represents the maximum slope of the linear regression. Typical options include: `'mu.linfit'`, `'lambda.linfit'`, `'dY.linfit'`, `'mu.spline'`, `'dY.spline'`, `'mu.model'`, and `'A.model'`.

`smooth.dr`
: (Numeric) Smoothing parameter used in the spline fit by smooth.spline during dose response curve estimation. Usually (not necessesary) in (0; 1]. See documentation of smooth.spline for further details. Default: `NULL`.

`log.x.dr`
: (Logical) Indicates whether `ln(x+1)` should be applied to the concentration data of the dose response curves. Default: `FALSE`.

`log.y.dr`
: (Logical) Indicates whether `ln(y+1)` should be applied to the response data of the dose response curves. Default: `FALSE`.

`nboot.dr`
: (Numeric) Defines the number of bootstrap samples for EC50 estimation. Use `nboot.dr = 0` to disable bootstrapping. Default: `0`.

`report`
: (Character or NULL) Create a PDF (`'pdf'`) and/or HTML (`'html'`) report after running all computations. Define `NULL` if no report should be created. Default: (`c('pdf', 'html')`)

`out.dir`
: Character or `NULL` Define the name of a folder in which all result files are stored. If `NULL`, the folder will be named with a combination of 'GrowthResults_' and the current date and time.

`out.nm`
: Character or `NULL` Define the name of the report files. If `NULL`, the files will be named with a combination of 'GrowthReport_' and the current date and time.

`export.fig`
: (Logical) Export all figures created in the report as separate PNG and PDF files (`TRUE`) or not (`FALSE`). Only effective if `report != NULL`.

`export.res`
: (Logical) Create tab-separated TXT files containing calculated growth parameters and dose-response analysis results as well as an .RData file for the resulting `grofit` object.

`parallelize`
: Run linear fits and bootstrapping operations in parallel using all but one available processor cores

`...`
: Further arguments passed to the shiny app.

Details

Common response parameters used in dose-response analysis:Linear fit:- mu.linfit: Growth rate- lambda.linfit: Lag time- dY.linfit: Density increase- A.linfit: Maximum measurementSpline fit:- mu.spline: Growth rate- lambda.spline: Lag time- A.spline: Maximum measurement- dY.spline: Density increase- integral.spline: IntegralParametric fit:- mu.model: Growth rate- lambda.model: Lag time- A.model: Maximum measurement- integral.model: Integral'

Value

A grofit object that contains all computation results, compatible with various plotting functions of the QurvE package and with growth.report.

time	Raw time matrix passed to the function as time (if no grofit object is provided).
data	Raw growth dataframe passed to the function as data (if no grofit object is provided).
gcFit	gcFit object created with the call of growth.gcFit.
drFit	drFit object created with the call of growth.drFit.
expdesign	Experimental design table inherited from grodata or created from the identifier columns (columns 1-3) in data.
control	Object of class grofit.control created with the call of growth.control.

See Also

Other workflows: flFit(), growth.gcFit()

Other growth fitting functions: growth.drFit(), growth.gcBootSpline(), growth.gcFitLinear(), growth.gcFitModel(), growth.gcFitSpline(), growth.gcFit()

Other dose-response analysis functions: flFit(), growth.drBootSpline(), growth.drFitSpline(), growth.gcFit()

Examples

```
# Create random growth data set
  rnd.data1 <- rdm.data(d = 35, mu = 0.8, A = 5, label = 'Test1')
  rnd.data2 <- rdm.data(d = 35, mu = 0.6, A = 4.5, label = 'Test2')

  rnd.data <- list()
  rnd.data[['time']] <- rbind(rnd.data1$time, rnd.data2$time)
  rnd.data[['data']] <- rbind(rnd.data1$data, rnd.data2$data)

  # Run growth curve analysis workflow
  res <- growth.workflow(time = rnd.data$time,
                         data = rnd.data$data,
                         fit.opt = 's',
                         ec50 = FALSE,
                         export.res = FALSE,
                         suppress.messages = TRUE,
                         parallelize = FALSE)

# Load custom dataset
  input <- read_data(data.growth = system.file('2-FMA_toxicity.csv', package = 'QurvE'))

  res <- growth.workflow(grodata = input,
                         fit.opt = 's',
                         ec50 = TRUE,
                         export.res = FALSE,
                         suppress.messages = TRUE,
```

```
                          parallelize = FALSE)

  plot(res)
```

`inflect` *Find indices of maxima an minima in a data series*

Description

Find indices of maxima an minima in a data series

Usage

```
inflect(x, threshold = 1)
```

Arguments

`x`	vector of values with minima and maxima
`threshold`	Threshold to consider minima or maxima

Value

a list with 1. a vector of minima and 2. a vector of maxima.

Author(s)

Evan Friedland

Examples

```
# Pick a desired threshold to plot up to
n <- 3
# Generate Data
randomwalk <- 100 + cumsum(rnorm(50, 0.2, 1)) # climbs upwards most of the time
bottoms <- lapply(1:n, function(x) inflect(randomwalk, threshold = x)$minima)
tops <- lapply(1:n, function(x) inflect(randomwalk, threshold = x)$maxima)
# Color functions
cf.1 <- grDevices::colorRampPalette(c('pink','red'))
cf.2 <- grDevices::colorRampPalette(c('cyan','blue'))
plot(randomwalk, type = 'l', main = 'Minima & Maxima\nVariable Thresholds')
for(i in 1:n){
  points(bottoms[[i]], randomwalk[bottoms[[i]]], pch = 16, col = cf.1(n)[i], cex = i/1.5)
}
for(i in 1:n){
  points(tops[[i]], randomwalk[tops[[i]]], pch = 16, col = cf.2(n)[i], cex = i/1.5)
}
legend('topleft', legend = c('Minima',1:n,'Maxima',1:n),
       pch = rep(c(NA, rep(16,n)), 2), col = c(1, cf.1(n),1, cf.2(n)),
       pt.cex =  c(rep(c(1, c(1:n) / 1.5), 2)), cex = .75, ncol = 2)
```

lm_parms *Helper functions for handling linear fits.*

Description

lm_window performs a linear regression with the Theil-Sen estimator on a subset of data.

Usage

```
lm_parms(m)

lm_window(x, y, i0, h = 5)
```

Arguments

m	linear model (lm) object
x	vector of independent variable (e.g. time).
y	vector of dependent variable (concentration of organisms).
i0	index of first value used for a window.
h	with of the window (number of data).

Value

linear model object of class lm (lm_window) resp. vector with parameters of the fit (lm_parms).

References

Hall, B. G., H. Acar and M. Barlow 2013. Growth Rates Made Easy. Mol. Biol. Evol. 31: 232-238 doi:10.1093/molbev/mst197

Examples

```
# Create random growth dataset
rnd.dataset <- rdm.data(d = 35, mu = 0.8, A = 5, label = "Test1")

# Extract time and growth data for single sample
time <- rnd.dataset$time[1,]
data <- as.numeric(rnd.dataset$data[1,-(1:3)]) # Remove identifier columns
data.log <- log(data/data[1])

# Perform linear fit on 8th window of size 8
linreg <- lm_window(time, data.log, 8, h=8)

summary(linreg)

lm_parms(linreg)
```

`low.integrate` *Function to estimate the area under a curve given as x and y(x) values*

Description

Function to estimate the area under a curve given as x and y(x) values

Usage

```
low.integrate(x, y)
```

Arguments

`x`	Numeric vector of x values.
`y`	Numeric vector of y values with the same length as `x`.

Details

The function uses the the R internal function `smooth.spline`.

Value

Numeric value: Area under the smoothed spline.

See Also

`smooth.spline`

Examples

```
# Create random growth dataset
rnd.dataset <- rdm.data(d = 35, mu = 0.8, A = 5, label = 'Test1')

# Extract time and growth data for single sample
time <- rnd.dataset$time[1,]
data <- as.numeric(rnd.dataset$data[1,-(1:3)]) # Remove identifier columns

plot(time, data)

print(low.integrate(time, data))
```

parse_data *Parse raw plate reader data and convert it to a format compatible with QurvE*

Description

parse_data takes a raw export file from a plate reader experiment (or similar device), extracts relevant information and parses it into the format required to run growth.workflow. If more than one read type is found the user is prompted to assign the correct reads to growth or fluorescence.

Usage

```
parse_data(
  data.file = NULL,
  map.file = NULL,
  software = c("Gen5", "Gen6", "Biolector", "Chi.Bio", "GrowthProfiler", "Tecan",
    "VictorNivo", "VictorX3"),
  convert.time = NULL,
  sheet.data = 1,
  sheet.map = 1,
  csvsep.data = ";",
  dec.data = ".",
  csvsep.map = ";",
  dec.map = ".",
  subtract.blank = TRUE,
  calib.growth = NULL,
  calib.fl = NULL,
  calib.fl2 = NULL,
  fl.normtype = c("growth", "fl2")
)
```

Arguments

data.file	(Character) A table file with extension '.xlsx', '.xls', '.csv', '.tsv', or '.txt' containing raw plate reader (or similar device) data.
map.file	(Character) A table file in column format with extension '.xlsx', '.xls', '.csv', '.tsv', or '.txt' with 'well', 'ID', 'replicate', and 'concentration' in the first row. Used to assign sample information to wells in a plate.
software	(Character) The name of the software/device used to export the plate reader data.
convert.time	(NULL or string) Convert time values with a formula provided in the form 'y = function(x)'. For example: convert.time = 'y = 24 * x'
sheet.data, sheet.map	(Numeric or Character) Number or name of the sheets in XLS or XLSX files containing experimental data or mapping information, respectively (*optional*).

`csvsep.data, csvsep.map`
: (Character) separator used in CSV data files (ignored for other file types). Default: `";"`

`dec.data, dec.map`
: (Character) decimal separator used in CSV, TSV or TXT files with measurements and mapping information, respectively.

`subtract.blank`
: (Logical) Shall blank values be subtracted from values within the same experiment (TRUE, the default) or not (FALSE).

`calib.growth, calib.fl, calib.fl2`
: (Character or `NULL`) Provide an equation in the form 'y = function(x)' (for example: 'y = x^2 * 0.3 - 0.5') to convert growth and fluorescence values. This can be used to, e.g., convert plate reader absorbance values into OD_{600} or fluorescence intensity into molecule concentrations. Caution!: When utilizing calibration, carefully consider whether or not blanks were subtracted to determine the calibration before selecting the input `subtract.blank = TRUE`.

`fl.normtype`
: (Character string) Normalize fluorescence values by either diving by `'growth'` or by fluorescence2 values (`'fl2'`).

Details

Mapping layout

well	ID	replicate	con
A1	Condition_A	1	
A2	Condition_A	2	
A3	Condition_A	3	
A4	Condition_B	1	
A5	Condition_B	2	
A6	Condition_B	3	
A7	Condition_A	1	
A8	Condition_A	2	
A9	Condition_A	3	
A10	Condition_B	1	
A11	Condition_B	2	
A12	Condition_B	3	
B1	Blank		
...	...	...	

Metadata provided as `map.file` needs to have the following layout:

Value

A `grodata` object suitable to run `growth.workflow`. See `read_data` for its structure.

Examples

```
if(interactive()){
grodata <- parse_data(data.file = system.file("fluorescence_test_Gen5.xlsx", package = "QurvE"),
                      sheet.data = 1,
                map.file = system.file("fluorescence_test_Gen5.xlsx", package = "QurvE"),
                      sheet.map = "mapping",
                      software = "Gen5",
                      convert.time = "y = x * 24", # convert days to hours
                      calib.growth = "y = x * 3.058") # convert absorbance to OD values
}
```

---

parse_Gen5Gen6 *Extract relevant data from a raw data export file generated with the "Gen5" or "Gen6" software.*

Description

Extract relevant data from a raw data export file generated with the "Gen5" or "Gen6" software.

Usage

```
parse_Gen5Gen6(input)
```

Arguments

input	A dataframe created by reading a table file with read_file

Value

a list of length two containing growth and/or fluorescence dataframes in the first and second element, respectively. The first column in these dataframes represents a time vector.

Examples

```
if(interactive()){
input <- read_file(filename = system.file("fluorescence_test_Gen5.xlsx", package = "QurvE") )
parsed <- parse_Gen5Gen6(input)
}
```

parse_victornivo — *Extract relevant data from a raw data export file generated from the software of Perkin Elmer's "Victor Nivo" plate readers.*

Description

Extract relevant data from a raw data export file generated from the software of Perkin Elmer's "Victor Nivo" plate readers.

Usage

```
parse_victornivo(input)
```

Arguments

input	A dataframe created by reading a table file with read_file

Value

a list of length two containing growth and/or fluorescence dataframes in the first and second element, respectively. The first column in these dataframes represents a time vector.

Examples

```
if(interactive()){
input <- read_file(filename = system.file("nivo_output.csv", package = "QurvE"), csvsep = "," )
parsed <- parse_victornivo(input)
}
```

parse_victorx3 — *Extract relevant data from a raw data export file generated from the software of Perkin Elmer's "Victor X3" plate readers.*

Description

Extract relevant data from a raw data export file generated from the software of Perkin Elmer's "Victor X3" plate readers.

Usage

```
parse_victorx3(input)
```

Arguments

input	A dataframe created by reading a table file with read_file

Value

a list of length two containing growth and/or fluorescence dataframes in the first and second element, respectively. The first column in these dataframes represents a time vector.

Examples

```
if(interactive()){
input <- read_file(filename = system.file("victorx3_output.txt", package = "QurvE") )
parsed <- parse_victorx3(input)
}
```

`plot.drBootSpline` *Generic plot function for* `gcBootSpline` *objects.*

Description

Generic plot function for `gcBootSpline` objects.

Usage

```
## S3 method for class 'drBootSpline'
plot(
  x,
  pch = 19,
  colData = 1,
  colSpline = "black",
  cex.point = 1,
  cex.lab = 1.5,
  cex.axis = 1.3,
  lwd = 2,
  plot = TRUE,
  export = FALSE,
  height = 7,
  width = 9,
  out.dir = NULL,
  combine = FALSE,
  ...
)
```

Arguments

`x`	A `drBootSpline` object created with `growth.drBootSpline` or stored within a `grofit` or `drFit` object created with `growth.workflow` or `growth.drFit`, respectively.
`pch`	(Numeric) Shape of the raw data symbols.
`colData`	(Numeric or Character) Color used to plot the raw data.

colSpline	(Numeric or Character) Color used to plot the splines.
cex.point	(Numeric) Size of the raw data points.
cex.lab	(Numeric) Font size of axis titles.
cex.axis	(Numeric) Font size of axis annotations.
lwd	(Numeric) Spline line width.
plot	(Logical) Show the generated plot in the Plots pane (TRUE) or not (FALSE).
export	(Logical) Export the generated plot as PDF and PNG files (TRUE) or not (FALSE).
height	(Numeric) Height of the exported image in inches.
width	(Numeric) Width of the exported image in inches.
out.dir	(Character) Name or path to a folder in which the exported files are stored. If NULL, a "Plots" folder is created in the current working directory to store the files in.
combine	(Logical) Indicate whether both dose-response curves and parameter plots shall be shown within the same window.
...	Further arguments to refine the generated base R plot.

Value

A plot with the all dose-response spline fits from the bootstrapping operation.

Examples

```
conc <- c(0, rev(unlist(lapply(1:18, function(x) 10*(2/3)^x))),10)
response <- c(1/(1+exp(-0.7*(4-conc[-20])))+stats::rnorm(19)/50, 0)

TestRun <- growth.drBootSpline(conc, response, drID = "test",
        control = growth.control(log.x.dr = TRUE, smooth.dr = 0.8, nboot.dr = 50))

print(summary(TestRun))
plot(TestRun, combine = TRUE)
```

---

plot.drFit *Generic plot function for* drFit *objects.*

Description

plot.drFit calls plot.drFitSpline for each group used in a dose-response analysis

Usage

```
## S3 method for class 'drFit'
plot(
  x,
  combine = TRUE,
  names = NULL,
  exclude.nm = NULL,
  pch = 16,
  cex.point = 2,
  basesize = 15,
  colors = NULL,
  lwd = 0.7,
  ec50line = TRUE,
  y.lim = NULL,
  x.lim = NULL,
  y.title = NULL,
  x.title = NULL,
  log.y = FALSE,
  log.x = FALSE,
  plot = TRUE,
  export = FALSE,
  height = NULL,
  width = NULL,
  out.dir = NULL,
  out.nm = NULL,
  ...
)
```

Arguments

x	object of class drFit, created with growth.drFit.
combine	(Logical) Combine the dose-response analysis results of all conditions into a single plot (TRUE) or not (FALSE).
names	(String or vector of strings) Define conditions to combine into a single plot (if combine = TRUE). Partial matches with sample/group names are accepted. If NULL, all samples are considered. Note: Ensure to use unique substrings to extract groups of interest. If the name of one condition is included in its entirety within the name of other conditions, it cannot be extracted individually.
exclude.nm	(String or vector of strings) Define conditions to exclude from the plot (if combine = TRUE). Partial matches with sample/group names are accepted.
pch	(Numeric) Shape of the raw data symbols.
cex.point	(Numeric) Size of the raw data points.
basesize	(Numeric) Base font size.
colors	(Numeric or character) Define colors for different conditions.
lwd	(Numeric) Line width of the individual splines.

ec50line	(Logical) Show pointed horizontal and vertical lines at the EC50 values (TRUE) or not (FALSE).
y.lim	(Numeric vector with two elements) Optional: Provide the lower (l) and upper (u) bounds on the y-axis as a vector in the form c(l, u). If only the lower or upper bound should be fixed, provide c(l, NA) or c(NA, u), respectively.
x.lim	(Numeric vector with two elements) Optional: Provide the lower (l) and upper (u) bounds on the x-axis as a vector in the form c(l, u). If only the lower or upper bound should be fixed, provide c(l, NA) or c(NA, u), respectively.
y.title	(Character) Optional: Provide a title for the y-axis.
x.title	(Character) Optional: Provide a title for the x-axis.
log.y	(Logical) Log-transform the y-axis of the plot (TRUE) or not (FALSE)?
log.x	(Logical) Log-transform the x-axis of the plot (TRUE) or not (FALSE)?
plot	(Logical) Show the generated plot in the Plots pane (TRUE) or not (FALSE).
export	(Logical) Export the generated plot as PDF and PNG files (TRUE) or not (FALSE).
height	(Numeric) Height of the exported image in inches.
width	(Numeric) Width of the exported image in inches.
out.dir	(Character) Name or path to a folder in which the exported files are stored. If NULL, a "Plots" folder is created in the current working directory to store the files in.
out.nm	(Character) The name of the PDF and PNG files if export = TRUE. If NULL, a name will be automatically generated including the chosen parameter.
...	Additional arguments. This has currently no effect and is only meant to fulfill the requirements of a generic function.

Value

One plot per condition tested in the dose-response analysis or a single plot showing all conditions if control = growth.control(dr.method = "spline") was used in growth.drFit and combine = TRUE.

Examples

```
# Create random growth data set
rnd.data1 <- rdm.data(d = 35, mu = 0.8, A = 5, label = "Test1")
rnd.data2 <- rdm.data(d = 35, mu = 0.6, A = 4.5, label = "Test2")

rnd.data <- list()
rnd.data[["time"]] <- rbind(rnd.data1$time, rnd.data2$time)
rnd.data[["data"]] <- rbind(rnd.data1$data, rnd.data2$data)

# Run growth curve analysis workflow
gcFit <- growth.gcFit(time = rnd.data$time,
                      data = rnd.data$data,
                      parallelize = FALSE,
                      control = growth.control(fit.opt = "s",
```

```
                                                suppress.messages = TRUE))

# Perform dose-response analysis
drFit <- growth.drFit(gcTable = gcFit$gcTable,
                 control = growth.control(dr.parameter = "mu.spline"))

# Inspect results
summary(drFit)

plot(drFit)
```

`plot.drFitfl` *Generic plot function for* `drFitFL` *objects.*

Description

`drFitfl` calls `plot.drFitFLModel` for each group used in a dose-response analysis with `dr.method = "model"`

Usage

```
## S3 method for class 'drFitfl'
plot(
  x,
  ec50line = TRUE,
  log = c("xy"),
  pch = 1,
  broken = TRUE,
  bp,
  n.xbreaks,
  n.ybreaks,
  colSpline = 1,
  colData = 1,
  cex.point = 1,
  cex.lab = 1.5,
  cex.axis = 1.3,
  y.lim = NULL,
  x.lim = NULL,
  lwd = 2,
  plot = TRUE,
  export = FALSE,
  height = 7,
  width = 9,
  out.dir = NULL,
  ...
)
```

Arguments

x	object of class drFit, created with growth.drFit.
ec50line	(Logical) Show pointed horizontal and vertical lines at the EC50 values (TRUE) or not (FALSE).
log	(Character) String which contains '"x"' if the x axis is to be logarithmic, '"y"' if the y axis is to be logarithmic and '"xy"' or '"yx"' if both axes are to be logarithmic. The default is "x". The empty string "" yields the original axes.
pch	(Numeric) Shape of the raw data symbols.
broken	(Logical) If TRUE the x axis is broken provided this axis is logarithmic (using functionality in the CRAN package 'plotrix').
bp	(Numeric) Specifying the break point below which the dose is zero (the amount of stretching on the dose axis above zero in order to create the visual illusion of a logarithmic scale including 0). The default is the base-10 value corresponding to the rounded value of the minimum of the log10 values of all positive dose values. This argument is only working for logarithmic dose axes.
n.xbreaks	(Numeric) Number of breaks on the x-axis (if not log-transformed). The breaks are generated using pretty. Thus, the final number of breaks can deviate from the user input.
n.ybreaks	(Numeric) Number of breaks on the y-axis (if not log-transformed). The breaks are generated using pretty. Thus, the final number of breaks can deviate from the user input.
colSpline	(Numeric or character) Spline line colour.
colData	(Numeric or character) Contour color of the raw data circles.
cex.point	(Numeric) Size of the raw data points.
cex.lab	(Numeric) Font size of axis titles.
cex.axis	(Numeric) Font size of axis annotations.
y.lim	(Numeric vector with two elements) Optional: Provide the lower (l) and upper (u) bounds on the y-axis as a vector in the form c(l, u). If only the lower or upper bound should be fixed, provide c(l, NA) or c(NA, u), respectively.
x.lim	(Numeric vector with two elements) Optional: Provide the lower (l) and upper (u) bounds on the x-axis as a vector in the form c(l, u). If only the lower or upper bound should be fixed, provide c(l, NA) or c(NA, u), respectively.
lwd	(Numeric) Line width of the individual splines.
plot	(Logical) Show the generated plot in the Plots pane (TRUE) or not (FALSE).
export	(Logical) Export the generated plot as PDF and PNG files (TRUE) or not (FALSE).
height	(Numeric) Height of the exported image in inches.
width	(Numeric) Width of the exported image in inches.
out.dir	(Character) Name or path to a folder in which the exported files are stored. If NULL, a "Plots" folder is created in the current working directory to store the files in.
...	Additional arguments. This has currently no effect and is only meant to fulfill the requirements of a generic function.

Value

One plot per condition tested in the dose-response analysis (fl.drFit with control = fl.control(dr.method = "model")).

Examples

```
# load example dataset
input <- read_data(data.growth = system.file("lac_promoters_growth.txt", package = "QurvE"),
              data.fl = system.file("lac_promoters_fluorescence.txt", package = "QurvE"),
                   csvsep = "\t",
                   csvsep.fl = "\t")

# Define fit controls
control <- fl.control(fit.opt = "s",
             x_type = "time", norm_fl = TRUE,
             dr.parameter = "max_slope.spline",
             dr.method = "model",
             suppress.messages = TRUE)

# Run curve fitting workflow
res <- flFit(fl_data = input$norm.fluorescence,
             time = input$time,
             parallelize = FALSE,
             control = control)

# Perform dose-response analysis with biosensor model
drFitfl <- fl.drFit(flTable = res$flTable, control = control)

plot(drFitfl)
```

---

plot.drFitFLModel *Generic plot function for* drFitFLModel *objects.*

Description

Generic plot function for drFitFLModel objects.

Usage

```
## S3 method for class 'drFitFLModel'
plot(
  x,
  ec50line = TRUE,
  broken = TRUE,
  bp,
  n.xbreaks,
  n.ybreaks,
  log = c("xy"),
```

```
  pch = 1,
  colSpline = 1,
  colData = 1,
  cex.point = 1,
  cex.lab = 1.5,
  cex.axis = 1.3,
  y.lim = NULL,
  x.lim = NULL,
  lwd = 2,
  plot = TRUE,
  export = FALSE,
  height = 7,
  width = 9,
  out.dir = NULL,
  ...
)
```

Arguments

x	Object of class drFitFLModel, created with fl.drFitModel.
ec50line	(Logical) Show pointed horizontal and vertical lines at the EC50 value (TRUE) or not (FALSE).
broken	(Logical) If TRUE the x axis is broken provided this axis is logarithmic (using functionality in the CRAN package 'plotrix').
bp	(Numeric) Specifying the break point below which the dose is zero (the amount of stretching on the dose axis above zero in order to create the visual illusion of a logarithmic scale including 0). The default is the base-10 value corresponding to the rounded value of the minimum of the log10 values of all positive dose values. This argument is only working for logarithmic dose axes.
n.xbreaks	(Numeric) Number of breaks on the x-axis (if not log-transformed). The breaks are generated using pretty. Thus, the final number of breaks can deviate from the user input.
n.ybreaks	(Numeric) Number of breaks on the y-axis (if not log-transformed). The breaks are generated using pretty. Thus, the final number of breaks can deviate from the user input.#' @param pch (Numeric) Size of the raw data circles.
log	(Character) String which contains '"x"' if the x axis is to be logarithmic, '"y"' if the y axis is to be logarithmic and '"xy"' or '"yx"' if both axes are to be logarithmic. The default is "x". The empty string "" yields the original axes.
pch	(Numeric) Symbol used to plot data points.
colSpline	(Numeric or Character) Color used to plot the splines.
colData	(Numeric or Character) Color used to plot the raw data.
cex.point	(Numeric) Size of the raw data points.
cex.lab	(Numeric) Font size of axis titles.
cex.axis	(Numeric) Font size of axis annotations.

y.lim	(Numeric vector with two elements) Optional: Provide the lower (l) and upper (u) bounds on y-axis as a vector in the form c(l, u).
x.lim	(Numeric vector with two elements) Optional: Provide the lower (l) and upper (u) bounds on the x-axis as a vector in the form c(l, u).
lwd	(Numeric) Line width.
plot	(Logical) Show the generated plot in the Plots pane (TRUE) or not (FALSE).
export	(Logical) Export the generated plot as PDF and PNG files (TRUE) or not (FALSE).
height	(Numeric) Height of the exported image in inches.
width	(Numeric) Width of the exported image in inches.
out.dir	(Character) Name or path to a folder in which the exported files are stored. If NULL, a "Plots" folder is created in the current working directory to store the files in.
...	Further arguments to refine the generated base R plot.

Value

A plot with the biosensor dose-response model fit.

Examples

```
# Create concentration values via a serial dilution
conc <- c(0, rev(unlist(lapply(1:18, function(x) 10*(2/3)^x))),10)

# Simulate response values via biosensor equation
response <- biosensor.eq(conc, y.min = 110, y.max = 6000, K = 0.5, n = 2) +
            0.01*6000*rnorm(10)

# Perform fit
TestRun <- fl.drFitModel(conc, response, drID = "test", control = fl.control())

print(summary(TestRun))
plot(TestRun)
```

---

plot.drFitModel *Generic plot function for* drFitModel *objects.*

Description

Generic plot function for drFitModel objects.

Usage

```
## S3 method for class 'drFitModel'
plot(
  x,
  type = c("confidence", "all", "bars", "none", "obs", "average"),
  ec50line = TRUE,
  add = FALSE,
  broken = TRUE,
  bp,
  gridsize = 200,
  log = "x",
  n.xbreaks,
  n.ybreaks,
  x.lim,
  y.lim,
  pch = 1,
  cex.point,
  cex.axis = 1,
  cex.lab = 1.3,
  col = 1,
  lwd = 2,
  lty = 2,
  xlab,
  ylab,
  legend = TRUE,
  legendText,
  legendPos,
  cex.legend = NULL,
  plot = TRUE,
  export = FALSE,
  height = 7,
  width = 9,
  out.dir = NULL,
  ...
)
```

Arguments

x	object of class drFitModel, created with growth.drFitModel.
type	(Character) Specify how to plot the data. There are currently 5 options: "average" (averages and fitted curve(s); default), "none" (only the fitted curve(s)), "obs" (only the data points), "all" (all data points and fitted curve(s)), "bars" (averages and fitted curve(s) with model-based standard errors (see Details)), and "confidence" (confidence bands for fitted curve(s)).
ec50line	(Logical) Show pointed horizontal and vertical lines at the EC50 values (TRUE) or not (FALSE).
add	(Logical) If TRUE then add to already existing plot.

broken	(Logical) If TRUE the x axis is broken provided this axis is logarithmic (using functionality in the CRAN package 'plotrix').
bp	(Numeric) Specifying the break point below which the dose is zero (the amount of stretching on the dose axis above zero in order to create the visual illusion of a logarithmic scale including 0). The default is the base-10 value corresponding to the rounded value of the minimum of the log10 values of all positive dose values. This argument is only working for logarithmic dose axes.
gridsize	(Numeric) Number of points in the grid used for plotting the fitted curves.
log	(Character) String which contains '"x"' if the x axis is to be logarithmic, '"y"' if the y axis is to be logarithmic and '"xy"' or '"yx"' if both axes are to be logarithmic. The default is "x". The empty string "" yields the original axes.
n.xbreaks	(Numeric) Number of breaks on the x-axis (if not log-transformed). The breaks are generated using `pretty`. Thus, the final number of breaks can deviate from the user input.
n.ybreaks	(Numeric) Number of breaks on the y-axis (if not log-transformed). The breaks are generated using `pretty`. Thus, the final number of breaks can deviate from the user input.
x.lim	(Numeric vector with two elements) Optional: Provide the lower (`l`) and upper (`u`) bounds on the x-axis of both growth curve and derivative plots as a vector in the form `c(l, u)`. If only the lower or upper bound should be fixed, provide `c(l, NA)` or `c(NA, u)`, respectively.
y.lim	(Numeric vector with two elements) Optional: Provide the lower (`l`) and upper (`u`) bounds on y-axis of the growth curve plot as a vector in the form `c(l, u)`. If only the lower or upper bound should be fixed, provide `c(l, NA)` or `c(NA, u)`, respectively.
pch	(Numeric) Symbol used to plot data points.
cex.point	(Numeric) Size of the raw data points.
cex.axis	(Numeric) Font size of axis annotations.
cex.lab	(Numeric) Font size of axis titles.
col	(Logical or a vector of colors) If `TRUE` default colours are used. If `FALSE` (default) no colors are used.
lwd	(Numeric) Line width.
lty	(Numeric) Specify the line type.
xlab	(Character) An optional label for the x axis.
ylab	(Character) An optional label for the y axis.
legend	(Logical) If `TRUE` a legend is displayed.
legendText	(Character) Specify the legend text (the position of the upper right corner of the legend box).
legendPos	(Numeric) Vector of length 2 giving the position of the legend.
cex.legend	numeric specifying the legend text size.
plot	(Logical) Show the generated plot in the `Plots` pane (`TRUE`) or not (`FALSE`).
export	(Logical) Export the generated plot as PDF and PNG files (`TRUE`) or not (`FALSE`).

height	(Numeric) Height of the exported image in inches.
width	(Numeric) Width of the exported image in inches.
out.dir	(Character) Name or path to a folder in which the exported files are stored. If NULL, a "Plots" folder is created in the current working directory to store the files in.
...	Additional arguments. This has currently no effect and is only meant to fulfill the requirements of a generic function.

Value

A plot with the dose-response model fit.

References

Christian Ritz, Florent Baty, Jens C. Streibig, Daniel Gerhard (2015). *Dose-Response Analysis Using R*. PLoS ONE 10(12): e0146021. DOI: 10.1371/journal.pone.0146021

Examples

```
conc <- c(0, rev(unlist(lapply(1:18, function(x) 10*(2/3)^x))),10)
response <- c(1/(1+exp(-0.7*(4-conc[-20])))+stats::rnorm(19)/50, 0)

TestRun <- growth.drFitModel(conc, response, drID = "test")

print(summary(TestRun))
plot(TestRun)
```

---

plot.drFitSpline *Generic plot function for* drFitSpline *objects.*

Description

plot.drFitSpline generates the spline fit plot for response-parameter vs. concentration data

Usage

```
## S3 method for class 'drFitSpline'
plot(
  x,
  add = FALSE,
  ec50line = TRUE,
  log = "",
  pch = 16,
  colSpline = 1,
  colData = 1,
  cex.point = 1,
  cex.lab = 1.5,
```

```
  cex.axis = 1.3,
  y.lim = NULL,
  x.lim = NULL,
  y.title = NULL,
  x.title = NULL,
  lwd = 2,
  plot = TRUE,
  export = FALSE,
  height = 7,
  width = 9,
  out.dir = NULL,
  ...
)
```

Arguments

x	object of class drFitSpline, created with growth.drFitSpline.
add	(Logical) Shall the fitted spline be added to an existing plot? TRUE is used internally by plot.drBootSpline.
ec50line	(Logical) Show pointed horizontal and vertical lines at the EC50 value (TRUE) or not (FALSE).
log	("x", "y", or "xy") Display the x- or y-axis on a logarithmic scale.
pch	(Numeric) Shape of the raw data symbols.
colSpline	(Numeric or character) Spline line colour.
colData	(Numeric or character) Contour color of the raw data circles.
cex.point	(Numeric) Size of the raw data symbols.
cex.lab	(Numeric) Font size of axis titles.
cex.axis	(Numeric) Font size of axis annotations.
y.lim	(Numeric vector with two elements) Optional: Provide the lower (l) and upper (u) bounds on the y-axis as a vector in the form c(l, u). If only the lower or upper bound should be fixed, provide c(l, NA) or c(NA, u), respectively.
x.lim	(Numeric vector with two elements) Optional: Provide the lower (l) and upper (u) bounds on the x-axis as a vector in the form c(l, u). If only the lower or upper bound should be fixed, provide c(l, NA) or c(NA, u), respectively.
y.title	(Character) Optional: Provide a title for the y-axis.
x.title	(Character) Optional: Provide a title for the x-axis.
lwd	(Numeric) Line width of spline.
plot	(Logical) Show the generated plot in the Plots pane (TRUE) or not (FALSE).
export	(Logical) Export the generated plot as PDF and PNG files (TRUE) or not (FALSE).
height	(Numeric) Height of the exported image in inches.
width	(Numeric) Width of the exported image in inches.
out.dir	(Character) Name or path to a folder in which the exported files are stored. If NULL, a "Plots" folder is created in the current working directory to store the files in.
...	Further arguments to refine the generated base R plot.

Value

A plot with the nonparametric dose-response fit.

Examples

```
conc <- c(0, rev(unlist(lapply(1:18, function(x) 10*(2/3)^x))),10)
response <- c(1/(1+exp(-0.7*(4-conc[-20])))+stats::rnorm(19)/50, 0)

TestRun <- growth.drFitSpline(conc, response, drID = "test",
                    control = growth.control(log.x.dr = TRUE, smooth.dr = 0.8))

print(summary(TestRun))
plot(TestRun)
```

---

plot.dr_parameter *Compare calculated dose-response parameters between conditions.*

Description

`plot.dr_parameter` gathers parameters from the results of a dose-response analysis and compares a chosen parameter between each condition in a column plot. Error bars represent the 95% confidence interval (only shown for > 2 replicates).

Usage

```
## S3 method for class 'dr_parameter'
plot(
  x,
  param = c("EC50", "EC50.Estimate", "y.max", "y.min", "fc", "K", "n", "yEC50",
    "drboot.meanEC50", "drboot.meanEC50y", "EC50.orig", "yEC50.orig"),
  names = NULL,
  exclude.nm = NULL,
  basesize = 12,
  reference.nm = NULL,
  label.size = NULL,
  plot = TRUE,
  export = FALSE,
  height = 7,
  width = NULL,
  out.dir = NULL,
  out.nm = NULL,
  ...
)
```

Arguments

x	A grofit, drFit, drTable, or flFitRes object obtained with growth.workflow, growth.drFit, fl.drFit, or fl.workflow.
param	(Character) The parameter used to compare different sample groups. Any name of a column containing numeric values in gcTable (which is stored within grofit or gcFit objects) can be used as input. Useful options are: 'y.max', 'y.min', 'fc', 'K', or 'n' for fluorescence dose-response analyses with dr.type = 'model' in the control argument, or 'EC50', 'yEC50', 'drboot.meanEC50', 'drboot.meanEC50y'.
names	(String or vector of strings) Define groups to combine into a single plot. Partial matches with sample/group names are accepted. If NULL, all samples are considered. Note: Ensure to use unique substrings to extract groups of interest. If the name of one condition is included in its entirety within the name of other conditions, it cannot be extracted individually.
exclude.nm	(String or vector of strings) Define groups to exclude from the plot. Partial matches with sample/group names are accepted.
basesize	(Numeric) Base font size.
reference.nm	(Character) Name of the reference condition, to which parameter values are normalized. Partially matching strings are tolerated as long as they can uniquely identify the condition.
label.size	(Numeric) Font size for sample labels below x-axis.
plot	(Logical) Show the generated plot in the Plots pane (TRUE) or not (FALSE). If FALSE, a ggplot object is returned.
export	(Logical) Export the generated plot as PDF and PNG files (TRUE) or not (FALSE).
height	(Numeric) Height of the exported image in inches.
width	(Numeric) Width of the exported image in inches.
out.dir	(Character) Name or path to a folder in which the exported files are stored. If NULL, a "Plots" folder is created in the current working directory to store the files in.
out.nm	(Character) The name of the PDF and PNG files if export = TRUE. If NULL, a name will be automatically generated including the chosen parameter.
...	Additional arguments. This has currently no effect and is only meant to fulfill the requirements of a generic function.

Value

A column plot comparing a selected parameter of a dose-response analysis between tested conditions.

Examples

```
# Create random growth data set
rnd.data1 <- rdm.data(d = 35, mu = 0.8, A = 5, label = "Test1")
rnd.data2 <- rdm.data(d = 35, mu = 0.6, A = 4.5, label = "Test2")
```

```
rnd.data <- list()
rnd.data[["time"]] <- rbind(rnd.data1$time, rnd.data2$time)
rnd.data[["data"]] <- rbind(rnd.data1$data, rnd.data2$data)

# Run growth curve analysis workflow
gcFit <- growth.gcFit(time = rnd.data$time,
                      data = rnd.data$data,
                      parallelize = FALSE,
                      control = growth.control(fit.opt = "s",
                                               suppress.messages = TRUE))

# Perform dose-response analysis
drFit <- growth.drFit(gcTable = gcFit$gcTable,
            control = growth.control(dr.parameter = "mu.spline"))

plot.dr_parameter(drFit, param = 'EC50')
```

`plot.dual` *Compare fluorescence and growth over time*

Description

`plot.dual` creates a two-panel plot in which fluorescence or growth values are shown over time, allowing for the identification of, e.g., expression patterns in different growth stages.

Usage

```
## S3 method for class 'dual'
plot(
  x,
  fluorescence = c("fl", "norm.fl"),
  IDs = NULL,
  names = NULL,
  conc = NULL,
  mean = TRUE,
  exclude.nm = NULL,
  exclude.conc = NULL,
  log.y.growth = FALSE,
  log.y.fl = FALSE,
  n.ybreaks = 6,
  colors = NULL,
  color_groups = TRUE,
 group_pals = c("Green", "Orange", "Purple", "Magenta", "Grey", "Blue", "Grey", "Red",
    "Cyan", "Brown", "Mint"),
  basesize = 20,
```

```
  y.lim.growth = NULL,
  y.lim.fl = NULL,
  x.lim = NULL,
  x.title = NULL,
  y.title.growth = NULL,
  y.title.fl = NULL,
  lwd = 1.1,
  legend.position = "bottom",
  legend.ncol = 2,
  plot = TRUE,
  export = FALSE,
  height = NULL,
  width = NULL,
  out.dir = NULL,
  out.nm = NULL,
  ...
)
```

Arguments

x	A flFit, flFitRes, or grodata object created with flFit, fl.workflow or read_data
fluorescence	(Character) Indicate, which type of fluorescence data should be displayed.
IDs	(String or vector of strings) Define samples or groups (if mean = TRUE) to combine into a single plot based on exact matches with entries in the label or condition columns of grofit$expdesign.
names	(String or vector of strings) Define groups to combine into a single plot. Partial matches with sample/group names are accepted. If NULL, all samples are considered. Note: Ensure to use unique substrings to extract groups of interest. If the name of one condition is included in its entirety within the name of other conditions, it cannot be extracted individually.
conc	(Numeric or numeric vector) Define concentrations to combine into a single plot. If NULL, all concentrations are considered. Note: Ensure to use unique concentration values to extract groups of interest. If the concentration value of one condition is included in its entirety within the name of other conditions (e.g., the dataset contains '1', '10', and '100', code = 10 will select both '10 and '100'), it cannot be extracted individually.
mean	(Logical) Display the mean and standard deviation of groups with replicates (TRUE) or plot each sample individually (FALSE)?
exclude.nm	(String or vector of strings) Define groups to exclude from the plot. Partial matches with sample/group names are accepted.
exclude.conc	(Numeric or numeric vector) Define concentrations to exclude from the plot.
log.y.growth	(Logical) Log-transform the y-axis of the growth plot (TRUE) or not (FALSE)?
log.y.fl	(Logical) Log-transform the y-axis of the fluorescence plot (TRUE) or not (FALSE)?
n.ybreaks	(Numeric) Number of breaks on the y-axis. The breaks are generated using scales::pretty_breaks. Thus, the final number of breaks can deviate from the user input.

colors	(vector of strings) Define a color palette used to draw the plots. If NULL, default palettes are chosen based on the number of groups/samples within the plot. Note: The number of provided colors should at least match the number of groups/samples.
color_groups	(Logical) Shall samples within the same group but with different concentrations be shown in different shades of the same color?
group_pals	(String vector) Define the colors used to display sample groups with identical concentrations. The number of selected color palettes must be at least the number of displayed groups. The order of the chosen palettes corresponds to the oder of conditions in the legend. Available options: "Green", "Oranges", "Purple", "Cyan", "Grey", "Red", "Blue", and "Magenta".
basesize	(Numeric) Base font size.
y.lim.growth	(Numeric vector with two elements) Optional: Provide the lower (l) and upper (u) bounds of the y-axis of the growth plot as a vector in the form c(l, u). If only the lower or upper bound should be fixed, provide c(l, NA) or c(NA, u), respectively.
y.lim.fl	(Numeric vector with two elements) Optional: Provide the lower (l) and upper (u) bounds of the y-axis of the fluorescence plot as a vector in the form c(l, u).
x.lim	(Numeric vector with two elements) Optional: Provide the lower (l) and upper (u) bounds of the x-axis of both fluorescence and growth plots as a vector in the form c(l, u). If only the lower or upper bound should be fixed, provide c(l, NA) or c(NA, u), respectively.
x.title	(Character) Optional: Provide a title for the x-axis of both growth curve and derivative plots.
y.title.growth	(Character) Optional: Provide a title for the y-axis of the growth plot.
y.title.fl	(Character) Optional: Provide a title for the y-axis of the fluorescence plot.
lwd	(Numeric) Line width of the individual plots.
legend.position	(Character) Position of the legend. One of "bottom", "top", "left", "right".
legend.ncol	(Numeric) Number of columns in the legend.
plot	(Logical) Show the generated plot in the Plots pane (TRUE) or not (FALSE). If FALSE, a ggplot object is returned.
export	(Logical) Export the generated plot as PDF and PNG files (TRUE) or not (FALSE).
height	(Numeric) Height of the exported image in inches.
width	(Numeric) Width of the exported image in inches.
out.dir	(Character) Name or path to a folder in which the exported files are stored. If NULL, a "Plots" folder is created in the current working directory to store the files in.
out.nm	(Character) The name of the PDF and PNG files if export = TRUE. If NULL, a name will be automatically generated including the chosen parameter.
...	Additional arguments. This has currently no effect and is only meant to fulfill the requirements of a generic function.

Value

A two-panel plot, showing raw fluorescence (`fluorescence = "fl"`) or normalized fluorescence (`fluorescence = "norm.fl"`) over time in the top panel, and growth over time in the bottom panel.

Examples

```
# load example dataset
input <- read_data(data.growth = system.file("lac_promoters_growth.txt", package = "QurvE"),
              data.fl = system.file("lac_promoters_fluorescence.txt", package = "QurvE"),
                   csvsep = "\t",
                   csvsep.fl = "\t")

# Run workflow
res <- fl.workflow(grodata = input, ec50 = FALSE, fit.opt = "s",
                   x_type = "time", norm_fl = TRUE,
                   dr.parameter = "max_slope.spline",
                   suppress.messages = TRUE,
                   parallelize = FALSE)

plot.dual(res, legend.ncol = 3, basesize = 15)
```

---

plot.flBootSpline *Generic plot function for* `flBootSpline` *objects.*

Description

Generic plot function for `flBootSpline` objects.

Usage

```
## S3 method for class 'flBootSpline'
plot(
  x,
  pch = 1,
  colData = 1,
  deriv = TRUE,
  colSpline = "dodgerblue3",
  cex.point = 1,
  cex.lab = 1.5,
  cex.axis = 1.3,
  lwd = 2,
  y.lim = NULL,
  x.lim = NULL,
  y.lim.deriv = NULL,
  plot = TRUE,
  export = FALSE,
```

```
  height = 7,
  width = 9,
  out.dir = NULL,
  combine = FALSE,
  ...
)
```

Arguments

x	Object of class flBootSpline, created with flBootSpline.
pch	(Numeric) Size of the raw data circles.
colData	(Numeric or Character) Color used to plot the raw data.
deriv	(Logical) Show the derivatives (i.e., slope) over time in a secondary plot (TRUE) or not (FALSE).
colSpline	(Numeric or Character) Color used to plot the splines.
cex.point	(Numeric) Size of the raw data points.
cex.lab	(Numeric) Font size of axis titles.
cex.axis	(Numeric) Font size of axis annotations.
lwd	(Numeric) Spline line width.
y.lim	(Numeric vector with two elements) Optional: Provide the lower (l) and upper (u) bounds on y-axis of the fluorescence curve plot as a vector in the form c(l, u). If only the lower or upper bound should be fixed, provide c(l, NA) or c(NA, u), respectively.
x.lim	(Numeric vector with two elements) Optional: Provide the lower (l) and upper (u) bounds on the x-axis of both fluorescence curve and derivative plots as a vector in the form c(l, u). If only the lower or upper bound should be fixed, provide c(l, NA) or c(NA, u), respectively.
y.lim.deriv	(Numeric vector with two elements) Optional: Provide the lower (l) and upper (u) bounds on the y-axis of the derivative plot as a vector in the form c(l, u). If only the lower or upper bound should be fixed, provide c(l, NA) or c(NA, u), respectively.
plot	(Logical) Show the generated plot in the Plots pane (TRUE) or not (FALSE).
export	(Logical) Export the generated plot as PDF and PNG files (TRUE) or not (FALSE).
height	(Numeric) Height of the exported image in inches.
width	(Numeric) Width of the exported image in inches.
out.dir	(Character) Name or path to a folder in which the exported files are stored. If NULL, a "Plots" folder is created in the current working directory to store the files in.
combine	(Logical) Indicate whether both growth curves and parameter plots shall be shown within the same window.
...	Additional arguments. This has currently no effect and is only meant to fulfill the requirements of a generic function.

Value

A single plot with the all spline fits from the bootstrapping operation and statistical distribution of parameters if `combine = TRUE` or separate plots for fits and parameter distributions (if `combine = FALSE`).

Examples

```
# load example dataset
input <- read_data(data.growth = system.file("lac_promoters_growth.txt", package = "QurvE"),
              data.fl = system.file("lac_promoters_fluorescence.txt", package = "QurvE"),
                   csvsep = "\t",
                   csvsep.fl = "\t")

# Extract time and normalized fluorescence data for single sample
time <- input$time[4,]
data <- input$norm.fluorescence[4,-(1:3)] # Remove identifier columns

# Perform linear fit
TestFit <- flBootSpline(time = time,
                        fl_data = data,
                        ID = "TestFit",
                        control = fl.control(fit.opt = "s", x_type = "time",
                        nboot.fl = 50))

plot(TestFit, combine = TRUE, lwd = 0.5)
```

---

plot.flFitLinear *Generic plot function for* `flcFittedLinear` *objects. Plot the results of a linear regression on ln-transformed data*

Description

`plot.flFitLinear` shows the results of a linear regression and visualizes raw data, data points included in the fit, the tangent obtained by linear regression, and the lag time.

Usage

```
## S3 method for class 'flFitLinear'
plot(
  x,
  log = "",
  which = c("fit", "diagnostics", "fit_diagnostics"),
  pch = 21,
  cex.point = 1,
  cex.lab = 1.5,
  cex.axis = 1.3,
  lwd = 2,
  color = "firebrick3",
```

```
  y.lim = NULL,
  x.lim = NULL,
  plot = TRUE,
  export = FALSE,
  height = ifelse(which == "fit", 7, 5),
  width = ifelse(which == "fit", 9, 9),
  out.dir = NULL,
  ...
)
```

Arguments

x	A `flFittedLinear` object created with `flFitLinear` or stored within a `flFitRes` or `flFit` object created with `fl.workflow` or `flFit`, respectively.
log	("x" or "y") Display the x- or y-axis on a logarithmic scale.
which	("fit" or "diagnostics") Display either the results of the linear fit on the raw data or statistical evaluation of the linear regression.
pch	(Numeric) Shape of the raw data symbols.
cex.point	(Numeric) Size of the raw data points.
cex.lab	(Numeric) Font size of axis titles.
cex.axis	(Numeric) Font size of axis annotations.
lwd	(Numeric) Line width.
color	(Character string) Enter color either by name (e.g., red, blue, coral3) or via their hexadecimal code (e.g., #AE4371, #CCFF00FF, #0066FFFF). A full list of colors available by name can be found at http://www.stat.columbia.edu/~tzheng/files/Rcolor.pdf
y.lim	(Numeric vector with two elements) Optional: Provide the lower (`l`) and upper (`u`) bounds on y-axis as a vector in the form `c(l, u)`.
x.lim	(Numeric vector with two elements) Optional: Provide the lower (`l`) and upper (`u`) bounds on the x-axis as a vector in the form `c(l, u)`.
plot	(Logical) Show the generated plot in the `Plots` pane (`TRUE`) or not (`FALSE`).
export	(Logical) Export the generated plot as PDF and PNG files (`TRUE`) or not (`FALSE`).
height	(Numeric) Height of the exported image in inches.
width	(Numeric) Width of the exported image in inches.
out.dir	(Character) Name or path to a folder in which the exported files are stored. If `NULL`, a "Plots" folder is created in the current working directory to store the files in.
...	Further arguments to refine the generated base R plot.

Value

A plot with the linear fit.

Examples

```
# load example dataset
input <- read_data(data.growth = system.file("lac_promoters_growth.txt", package = "QurvE"),
              data.fl = system.file("lac_promoters_fluorescence.txt", package = "QurvE"),
                   csvsep = "\t",
                   csvsep.fl = "\t")

# Extract time and normalized fluorescence data for single sample
time <- input$time[4,]
data <- input$norm.fluorescence[4,-(1:3)] # Remove identifier columns

# Perform linear fit
TestFit <- flFitLinear(time = time,
                       fl_data = data,
                       ID = "TestFit",
                       control = fl.control(fit.opt = "l", x_type = "time",
                       lin.R2 = 0.95, lin.RSD = 0.1,
                       lin.h = 20))

plot(TestFit)
```

`plot.flFitRes` *Combine different groups of samples into a single plot*

Description

Visualize fluorescence, normalized fluorescence, or spline fits of multiple sample groups in a single plot.

Usage

```
## S3 method for class 'flFitRes'
plot(
  x,
  data.type = c("spline", "raw", "norm.fl"),
  IDs = NULL,
  names = NULL,
  conc = NULL,
  mean = TRUE,
  exclude.nm = NULL,
  exclude.conc = NULL,
  log.y = FALSE,
  deriv = FALSE,
  n.ybreaks = 6,
  colors = NULL,
  color_groups = TRUE,
 group_pals = c("Green", "Orange", "Purple", "Magenta", "Grey", "Blue", "Grey", "Red",
    "Cyan", "Brown", "Mint"),
```

```
  basesize = 20,
  y.lim = NULL,
  x.lim = NULL,
  y.title = NULL,
  x.title = NULL,
  y.lim.deriv = NULL,
  y.title.deriv = NULL,
  lwd = 1.1,
  legend.position = "bottom",
  legend.ncol = 2,
  plot = TRUE,
  export = FALSE,
  height = NULL,
  width = NULL,
  out.dir = NULL,
  out.nm = NULL,
  ...
)

## S3 method for class 'flFit'
plot(
  x,
  data.type = c("spline", "raw", "norm.fl"),
  IDs = NULL,
  names = NULL,
  conc = NULL,
  mean = TRUE,
  exclude.nm = NULL,
  exclude.conc = NULL,
  log.y = FALSE,
  deriv = FALSE,
  n.ybreaks = 6,
  colors = NULL,
  color_groups = TRUE,
 group_pals = c("Green", "Orange", "Purple", "Magenta", "Grey", "Blue", "Grey", "Red",
    "Cyan", "Brown", "Mint"),
  basesize = 20,
  y.lim = NULL,
  x.lim = NULL,
  y.title = NULL,
  x.title = NULL,
  y.lim.deriv = NULL,
  y.title.deriv = NULL,
  lwd = 1.1,
  legend.position = "bottom",
  legend.ncol = 2,
  plot = TRUE,
  export = FALSE,
```

```
  height = NULL,
  width = NULL,
  out.dir = NULL,
  out.nm = NULL,
  ...
)
```

Arguments

x	A flFitRes, flFit, or grodata object created with fl.workflow containing fluorescence data.
data.type	(Character) Indicate, which type of fluorescence data should be displayed.
IDs	(String or vector of strings) Define samples or groups (if mean = TRUE) to combine into a single plot based on exact matches with entries in the label or condition columns of grofit$expdesign.
names	(String or vector of strings) Define groups to combine into a single plot. Partial matches with sample/group names are accepted. If NULL, all samples are considered. Note: Ensure to use unique substrings to extract groups of interest. If the name of one condition is included in its entirety within the name of other conditions, it cannot be extracted individually.
conc	(Numeric or numeric vector) Define concentrations to combine into a single plot. If NULL, all concentrations are considered. Note: Ensure to use unique concentration values to extract groups of interest. If the concentration value of one condition is included in its entirety within the name of other conditions (e.g., the dataset contains '1', '10', and '100', code = 10 will select both '10 and '100'), it cannot be extracted individually.
mean	(Logical) Display the mean and standard deviation of groups with replicates (TRUE) or plot each sample individually (FALSE)?
exclude.nm	(String or vector of strings) Define groups to exclude from the plot. Partial matches with sample/group names are accepted.
exclude.conc	(Numeric or numeric vector) Define concentrations to exclude from the plot.
log.y	(Logical) Log-transform the y-axis of the plot (TRUE) or not (FALSE)?
deriv	(Logical) Show derivatives over time in a separate panel below the plot (TRUE) or not (FALSE)?
n.ybreaks	(Numeric) Number of breaks on the y-axis. The breaks are generated using axisTicks(). Thus, the final number of breaks can deviate from the user input.
colors	(vector of strings) Define a color palette used to draw the plots. If NULL, default palettes are chosen based on the number of groups/samples within the plot. Note: The number of provided colors should at least match the number of groups/samples.
color_groups	(Logical) Shall samples within the same group but with different concentrations be shown in different shades of the same color?
group_pals	(String vector) Define the colors used to display sample groups with identical concentrations. The number of selected color palettes must be at least the number of displayed groups. The order of the chosen palettes corresponds to the oder

	of conditions in the legend. Available options: "Green", "Oranges", "Purple", "Cyan", "Grey", "Red", "Blue", and "Magenta".
basesize	(Numeric) Base font size.
y.lim	(Numeric vector with two elements) Optional: Provide the lower (l) and upper (u) bounds of the y-axis of the fluorescence curve plot as a vector in the form c(l, u). If only the lower or upper bound should be fixed, provide c(l, NA) or c(NA, u), respectively.
x.lim	(Numeric vector with two elements) Optional: Provide the lower (l) and upper (u) bounds of the x-axis of both fluorescence curve and derivative plots as a vector in the form c(l, u). If only the lower or upper bound should be fixed, provide c(l, NA) or c(NA, u), respectively.
y.title	(Character) Optional: Provide a title for the y-axis of the fluorescence curve plot.
x.title	(Character) Optional: Provide a title for the x-axis of both fluorescence curve and derivative plots.
y.lim.deriv	(Numeric vector with two elements) Optional: Provide the lower (l) and upper (u) bounds on the y-axis of the derivative plot as a vector in the form c(l, u). If only the lower or upper bound should be fixed, provide c(l, NA) or c(NA, u), respectively.
y.title.deriv	(Character) Optional: Provide a title for the y-axis of the derivative plot.
lwd	(Numeric) Line width of the individual plots.
legend.position	(Character) Position of the legend. One of "bottom", "top", "left", "right".
legend.ncol	(Numeric) Number of columns in the legend.
plot	(Logical) Show the generated plot in the Plots pane (TRUE) or not (FALSE). If FALSE, a ggplot object is returned.
export	(Logical) Export the generated plot as PDF and PNG files (TRUE) or not (FALSE).
height	(Numeric) Height of the exported image in inches.
width	(Numeric) Width of the exported image in inches.
out.dir	(Character) Name or path to a folder in which the exported files are stored. If NULL, a "Plots" folder is created in the current working directory to store the files in.
out.nm	(Character) The name of the PDF and PNG files if export = TRUE. If NULL, a name will be automatically generated including the chosen parameter.
...	Additional arguments. This has currently no effect and is only meant to fulfill the requirements of a generic function.

Value

A plot with all curves (nonparametric fits, raw fluorescence measurements, or raw normalized fluorescence over time) in a flFitRes object created with fl.workflow, with replicates combined by the group averages (if mean = TRUE) or not (mean = FALSE).

A plot with all curves (raw fluorescence measurements or raw normalized fluorescence over time) in a flFit object with flFit, with replicates combined by the group averages (if mean = TRUE) or not (mean = FALSE).

Examples

```
# load example dataset
input <- read_data(data.growth = system.file("lac_promoters_growth.txt", package = "QurvE"),
              data.fl = system.file("lac_promoters_fluorescence.txt", package = "QurvE"),
                   csvsep = "\t",
                   csvsep.fl = "\t")

# Run workflow
res <- fl.workflow(grodata = input, ec50 = FALSE, fit.opt = "s",
                   x_type = "time", norm_fl = TRUE,
                   dr.parameter = "max_slope.spline",
                   suppress.messages = TRUE,
                   parallelize = FALSE)

plot(res, legend.ncol = 3, basesize = 15)


# load example dataset
input <- read_data(data.growth = system.file("lac_promoters_growth.txt", package = "QurvE"),
               data.fl = system.file("lac_promoters_fluorescence.txt", package = "QurvE"),
                   csvsep = "\t",
                   csvsep.fl = "\t")

# Run curve fitting workflow
res <- flFit(fl_data = input$norm.fluorescence,
             time = input$time,
             parallelize = FALSE,
             control = fl.control(fit.opt = "s", suppress.messages = TRUE,
             x_type = "time", norm_fl = TRUE))

plot(res, legend.ncol = 3, basesize = 15)
```

`plot.flFitSpline` *Generic plot function for* `flFitSpline` *objects.*

Description

`plot.flFitSpline` generates the spline fit plot for a single sample.

Usage

```
## S3 method for class 'flFitSpline'
plot(
  x,
  add = FALSE,
  raw = TRUE,
```

```
  slope = TRUE,
  deriv = TRUE,
  spline = TRUE,
  log.y = FALSE,
  basesize = 16,
  pch = 1,
  colData = 1,
  colSpline = "dodgerblue3",
  cex.point = 2,
  lwd = 0.7,
  y.lim = NULL,
  x.lim = NULL,
  y.lim.deriv = NULL,
  n.ybreaks = 6,
  y.title = NULL,
  x.title = NULL,
  y.title.deriv = NULL,
  plot = TRUE,
  export = FALSE,
  width = 8,
  height = ifelse(deriv == TRUE, 8, 6),
  out.dir = NULL,
  ...
)
```

Arguments

x	Object of class `flFitSpline`, created with `flFitSpline`.
add	(Logical) Shall the fitted spline be added to an existing plot? `TRUE` is used internally by `plot.flBootSpline`.
raw	(Logical) Display raw growth as circles (`TRUE`) or not (`FALSE`).
slope	(Logical) Show the slope at the maximum slope (`TRUE`) or not (`FALSE`).
deriv	(Logical) Show the derivative (i.e., slope) over time in a secondary plot (`TRUE`) or not (`FALSE`).
spline	(Logical) Only for `add = TRUE`: add the current spline to the existing plot (`FALSE`).
log.y	(Logical) Log-transform the y-axis (`TRUE`) or not (`FALSE`).
basesize	(Numeric) Base font size.
pch	(Numeric) Symbol used to plot data points.
colData	(Numeric or character) Contour color of the raw data circles.
colSpline	(Numeric or character) Spline line colour.
cex.point	(Numeric) Size of the raw data points.
lwd	(Numeric) Spline line width.
y.lim	(Numeric vector with two elements) Optional: Provide the lower (`l`) and upper (`u`) bounds on y-axis of the fluorescence curve plot as a vector in the form `c(l, u)`. If only the lower or upper bound should be fixed, provide `c(l, NA)` or `c(NA, u)`, respectively.

x.lim	(Numeric vector with two elements) Optional: Provide the lower (l) and upper (u) bounds on the x-axis of both fluorescence curve and derivative plots as a vector in the form c(l, u). If only the lower or upper bound should be fixed, provide c(l, NA) or c(NA, u), respectively.
y.lim.deriv	(Numeric vector with two elements) Optional: Provide the lower (l) and upper (u) bounds on the y-axis of the derivative plot as a vector in the form c(l, u). If only the lower or upper bound should be fixed, provide c(l, NA) or c(NA, u), respectively.
n.ybreaks	(Numeric) Number of breaks on the y-axis. The breaks are generated using axisTicks(). Thus, the final number of breaks can deviate from the user input.
y.title	(Character) Optional: Provide a title for the y-axis of the growth curve plot.
x.title	(Character) Optional: Provide a title for the x-axis of both growth curve and derivative plots.
y.title.deriv	(Character) Optional: Provide a title for the y-axis of the derivative plot.
plot	(Logical) Show the generated plot in the Plots pane (TRUE) or not (FALSE). If FALSE, a ggplot object is returned.
export	(Logical) Export the generated plot as PDF and PNG files (TRUE) or not (FALSE).
width	(Numeric) Width of the exported image in inches.
height	(Numeric) Height of the exported image in inches.
out.dir	(Character) Name or path to a folder in which the exported files are stored. If NULL, a "Plots" folder is created in the current working directory to store the files in.
...	Additional arguments. This has currently no effect and is only meant to fulfill the requirements of a generic function.

Value

A plot with the nonparametric fit.

Examples

```
# load example dataset
input <- read_data(data.growth = system.file("lac_promoters_growth.txt", package = "QurvE"),
              data.fl = system.file("lac_promoters_fluorescence.txt", package = "QurvE"),
                   csvsep = "\t",
                   csvsep.fl = "\t")

# Extract time and normalized fluorescence data for single sample
time <- input$time[4,]
data <- input$norm.fluorescence[4,-(1:3)] # Remove identifier columns

# Perform linear fit
TestFit <- flFitSpline(time = time,
                       fl_data = data,
                       ID = "TestFit",
                       control = fl.control(fit.opt = "s", x_type = "time"))

plot(TestFit)
```

`plot.gcBootSpline` *Generic plot function for* `gcBootSpline` *objects.*

Description

Generic plot function for `gcBootSpline` objects.

Usage

```
## S3 method for class 'gcBootSpline'
plot(
  x,
  pch = 1,
  colData = 1,
  deriv = TRUE,
  colSpline = "dodgerblue3",
  cex.point = 1,
  cex.lab = 1.5,
  cex.axis = 1.3,
  lwd = 2,
  y.lim = NULL,
  x.lim = NULL,
  y.lim.deriv = NULL,
  plot = TRUE,
  export = FALSE,
  height = 7,
  width = 9,
  out.dir = NULL,
  combine = FALSE,
  ...
)
```

Arguments

`x`	object of class `gcBootSpline`, created with `growth.gcBootSpline`.
`pch`	(Numeric) Symbol used to plot data points.
`colData`	(Numeric or character) Contour color of the raw data circles.
`deriv`	(Logical) Show the derivatives (i.e., slope) over time in a secondary plot (`TRUE`) or not (`FALSE`).
`colSpline`	(Numeric or character) Spline line colour.
`cex.point`	(Numeric) Size of the raw data points.
`cex.lab`	(Numeric) Font size of axis titles.
`cex.axis`	(Numeric) Font size of axis annotations.
`lwd`	(Numeric) Spline line width.

y.lim	(Numeric vector with two elements) Optional: Provide the lower (l) and upper (u) bounds on y-axis of the growth curve plot as a vector in the form c(l, u). If only the lower or upper bound should be fixed, provide c(l, NA) or c(NA, u), respectively.
x.lim	(Numeric vector with two elements) Optional: Provide the lower (l) and upper (u) bounds on the x-axis of both growth curve and derivative plots as a vector in the form c(l, u). If only the lower or upper bound should be fixed, provide c(l, NA) or c(NA, u), respectively.
y.lim.deriv	(Numeric vector with two elements) Optional: Provide the lower (l) and upper (u) bounds on the y-axis of the derivative plot as a vector in the form c(l, u). If only the lower or upper bound should be fixed, provide c(l, NA) or c(NA, u), respectively.
plot	(Logical) Show the generated plot in the Plots pane (TRUE) or not (FALSE).
export	(Logical) Export the generated plot as PDF and PNG files (TRUE) or not (FALSE).
height	(Numeric) Height of the exported image in inches.
width	(Numeric) Width of the exported image in inches.
out.dir	(Character) Name or path to a folder in which the exported files are stored. If NULL, a "Plots" folder is created in the current working directory to store the files in.
combine	(Logical) Indicate whether both growth curves and parameter plots shall be shown within the same window.
...	Further arguments to refine the generated base R plot.

Value

A single plot with the all spline growth fits from the bootstrapping operation and statistical distribution of growth parameters if combine = TRUE or separate plots for growth fits and parameter distributions (if combine = FALSE).

Examples

```
# Create random growth dataset
rnd.dataset <- rdm.data(d = 35, mu = 0.8, A = 5, label = "Test1")

# Extract time and growth data for single sample
time <- rnd.dataset$time[1,]
data <- rnd.dataset$data[1,-(1:3)] # Remove identifier columns

# Introduce some noise into the measurements
data <- data + stats::runif(97, -0.01, 0.09)

# Perform bootstrapping spline fit
TestFit <- growth.gcBootSpline(time, data, gcID = "TestFit",
             control = growth.control(fit.opt = "s", nboot.gc = 50))

plot(TestFit, combine = TRUE, lwd = 0.5)
```

`plot.gcFitLinear` *Generic plot function for* `gcFittedLinear` *objects. Plot the results of a linear regression on ln-transformed data*

Description

`plot.gcFitLinear` shows the results of a linear regression on log-transformed data and visualizes raw data, data points included in the fit, the tangent obtained by linear regression, and the lag time.

Usage

```
## S3 method for class 'gcFitLinear'
plot(
  x,
  log = "y",
  which = c("fit", "diagnostics", "fit_diagnostics"),
  pch = 21,
  cex.point = 1,
  cex.lab = 1.5,
  cex.axis = 1.3,
  lwd = 2,
  color = "firebrick3",
  y.lim = NULL,
  x.lim = NULL,
  plot = TRUE,
  export = FALSE,
  height = ifelse(which == "fit", 7, 5),
  width = ifelse(which == "fit", 9, 9),
  out.dir = NULL,
  ...
)
```

Arguments

`x`	A `gcFittedLinear` object created with `growth.gcFitLinear` or stored within a `grofit` or `gcFit` object created with `growth.workflow` or `growth.gcFit`, respectively.
`log`	("x" or "y") Display the x- or y-axis on a logarithmic scale.
`which`	("fit" or "diagnostics") Display either the results of the linear fit on the raw data or statistical evaluation of the linear regression.
`pch`	(Numeric) Shape of the raw data symbols.
`cex.point`	(Numeric) Size of the raw data points.
`cex.lab`	(Numeric) Font size of axis titles.
`cex.axis`	(Numeric) Font size of axis annotations.
`lwd`	(Numeric) Line width.

color	(Character string) Enter color either by name (e.g., red, blue, coral3) or via their hexadecimal code (e.g., #AE4371, #CCFF00FF, #0066FFFF). A full list of colors available by name can be found at http://www.stat.columbia.edu/~tzheng/files/Rcolor.pdf
y.lim	(Numeric vector with two elements) Optional: Provide the lower (l) and upper (u) bounds on y-axis as a vector in the form c(l, u).
x.lim	(Numeric vector with two elements) Optional: Provide the lower (l) and upper (u) bounds on the x-axis as a vector in the form c(l, u).
plot	(Logical) Show the generated plot in the Plots pane (TRUE) or not (FALSE).
export	(Logical) Export the generated plot as PDF and PNG files (TRUE) or not (FALSE).
height	(Numeric) Height of the exported image in inches.
width	(Numeric) Width of the exported image in inches.
out.dir	(Character) Name or path to a folder in which the exported files are stored. If NULL, a "Plots" folder is created in the current working directory to store the files in.
...	Further arguments to refine the generated base R plot.

Value

A plot with the linear fit.

Examples

```
# Create random growth dataset
rnd.dataset <- rdm.data(d = 35, mu = 0.8, A = 5, label = "Test1")

# Extract time and growth data for single sample
time <- rnd.dataset$time[1,]
data <- rnd.dataset$data[1,-(1:3)] # Remove identifier columns

# Perform linear fit
TestFit <- growth.gcFitLinear(time, data, gcID = "TestFit",
                 control = growth.control(fit.opt = "l"))

plot(TestFit)
```

---

plot.gcFitModel *Generic plot function for* gcFitModel *objects.*

Description

Plot the results of a parametric model fit on growth vs. time data

Usage

```
## S3 method for class 'gcFitModel'
plot(
  x,
  raw = TRUE,
  pch = 1,
  colData = 1,
  equation = TRUE,
  eq.size = 1,
  colModel = "forestgreen",
  basesize = 16,
  cex.point = 2,
  lwd = 0.7,
  x.lim = NULL,
  y.lim = NULL,
  n.ybreaks = 6,
  plot = TRUE,
  export = FALSE,
  height = 6,
  width = 8,
  out.dir = NULL,
  ...
)
```

Arguments

x	A gcFittedModel object created with growth.gcFitModel or stored within a grofit or gcFit object created with growth.workflow or growth.gcFit, respectively.
raw	(Logical) Show the raw data within the plot (TRUE) or not (FALSE).
pch	(Numeric) Symbol used to plot data points.
colData	(Numeric or Character) Color used to plot the raw data.
equation	(Logical) Show the equation of the fitted model within the plot (TRUE) or not (FALSE).
eq.size	(Numeric) Provide a value to scale the size of the displayed equation.
colModel	(Numeric or Character) Color used to plot the fitted model.
basesize	(Numeric) Base font size.
cex.point	(Numeric) Size of the raw data points.
lwd	(Numeric) Spline line width.
x.lim	(Numeric vector with two elements) Optional: Provide the lower (l) and upper (u) bounds on the x-axis as a vector in the form c(l, u). If only the lower or upper bound should be fixed, provide c(l, NA) or c(NA, u), respectively.
y.lim	(Numeric vector with two elements) Optional: Provide the lower (l) and upper (u) bounds on y-axis of the growth curve plot as a vector in the form c(l, u). If only the lower or upper bound should be fixed, provide c(l, NA) or c(NA, u), respectively.

n.ybreaks	(Numeric) Number of breaks on the y-axis. The breaks are generated using scales::pretty_breaks. Thus, the final number of breaks can deviate from the user input.
plot	(Logical) Show the generated plot in the Plots pane (TRUE) or not (FALSE). If FALSE, a ggplot object is returned.
export	(Logical) Export the generated plot as PDF and PNG files (TRUE) or not (FALSE).
height	(Numeric) Height of the exported image in inches.
width	(Numeric) Width of the exported image in inches.
out.dir	(Character) Name or path to a folder in which the exported files are stored. If NULL, a "Plots" folder is created in the current working directory to store the files in.
...	Further arguments to refine the generated ggplot2 plot.

Value

A plot with the parametric fit.

Examples

```
# Create random growth dataset
rnd.dataset <- rdm.data(d = 35, mu = 0.8, A = 5, label = "Test1")

# Extract time and growth data for single sample
time <- rnd.dataset$time[1,]
data <- rnd.dataset$data[1,-(1:3)] # Remove identifier columns

# Perform parametric fit
TestFit <- growth.gcFitModel(time, data, gcID = "TestFit",
                 control = growth.control(fit.opt = "m"))

plot(TestFit, basesize = 18, eq.size = 1.5)
```

---

plot.gcFitSpline *Generic plot function for* gcFitSpline *objects.*

Description

plot.gcFitSpline generates the spline fit plot for a single sample.

Usage

```
## S3 method for class 'gcFitSpline'
plot(
  x,
  add = FALSE,
  raw = TRUE,
```

```
  slope = TRUE,
  deriv = TRUE,
  spline = TRUE,
  log.y = TRUE,
  pch = 1,
  colData = 1,
  colSpline = "dodgerblue3",
  basesize = 16,
  cex.point = 2,
  lwd = 0.7,
  y.lim = NULL,
  x.lim = NULL,
  y.lim.deriv = NULL,
  n.ybreaks = 6,
  y.title = NULL,
  x.title = NULL,
  y.title.deriv = NULL,
  plot = TRUE,
  export = FALSE,
  width = 8,
  height = ifelse(deriv == TRUE, 8, 6),
  out.dir = NULL,
  ...
)
```

Arguments

x	object of class gcFitSpline, created with growth.gcFitSpline.
add	(Logical) Shall the fitted spline be added to an existing plot? TRUE is used internally by plot.gcBootSpline.
raw	(Logical) Display raw growth as circles (TRUE) or not (FALSE).
slope	(Logical) Show the slope at the maximum growth rate (TRUE) or not (FALSE).
deriv	(Logical) Show the derivative (i.e., slope) over time in a secondary plot (TRUE) or not (FALSE).
spline	(Logical) Only for add = TRUE: add the current spline to the existing plot (FALSE).
log.y	(Logical) Log-transform the y-axis (TRUE) or not (FALSE).
pch	(Numeric) Symbol used to plot data points.
colData	(Numeric or character) Contour color of the raw data circles.
colSpline	(Numeric or character) Spline line colour.
basesize	(Numeric) Base font size.
cex.point	(Numeric) Size of the raw data points.
lwd	(Numeric) Spline line width.
y.lim	(Numeric vector with two elements) Optional: Provide the lower (l) and upper (u) bounds on y-axis of the growth curve plot as a vector in the form c(l, u). If only the lower or upper bound should be fixed, provide c(l, NA) or c(NA, u), respectively.

x.lim	(Numeric vector with two elements) Optional: Provide the lower (l) and upper (u) bounds on the x-axis of both growth curve and derivative plots as a vector in the form c(l, u). If only the lower or upper bound should be fixed, provide c(l, NA) or c(NA, u), respectively.
y.lim.deriv	(Numeric vector with two elements) Optional: Provide the lower (l) and upper (u) bounds on the y-axis of the derivative plot as a vector in the form c(l, u). If only the lower or upper bound should be fixed, provide c(l, NA) or c(NA, u), respectively.
n.ybreaks	(Numeric) Number of breaks on the y-axis. The breaks are generated using scales::pretty_breaks. Thus, the final number of breaks can deviate from the user input.
y.title	(Character) Optional: Provide a title for the y-axis of the growth curve plot.
x.title	(Character) Optional: Provide a title for the x-axis of both growth curve and derivative plots.
y.title.deriv	(Character) Optional: Provide a title for the y-axis of the derivative plot.
plot	(Logical) Show the generated plot in the Plots pane (TRUE) or not (FALSE). If FALSE, a ggplot object is returned.
export	(Logical) Export the generated plot as PDF and PNG files (TRUE) or not (FALSE).
width	(Numeric) Width of the exported image in inches.
height	(Numeric) Height of the exported image in inches.
out.dir	(Character) Name or path to a folder in which the exported files are stored. If NULL, a "Plots" folder is created in the current working directory to store the files in.
...	Further arguments to refine the generated base R plot (if add = TRUE.

Value

A plot with the nonparametric fit.

Examples

```
# Create random growth dataset
rnd.dataset <- rdm.data(d = 35, mu = 0.8, A = 5, label = "Test1")

# Extract time and growth data for single sample
time <- rnd.dataset$time[1,]
data <- rnd.dataset$data[1,-(1:3)] # Remove identifier columns

# Perform spline fit
TestFit <- growth.gcFitSpline(time, data, gcID = "TestFit",
                 control = growth.control(fit.opt = "s"))

plot(TestFit)
```

plot.grid *Plot a matrix of growth curve panels*

Description

plot.grid takes a grofit or flFitRes object and returns a facet grid of individual growth and fluorescence plots

Usage

```
## S3 method for class 'grid'
plot(
  x,
  data.type = c("spline", "raw", "norm.fl"),
  param = c("mu.linfit", "lambda.linfit", "dY.linfit", "A.linfit", "mu2.linfit",
   "lambda2.linfit", "mu.model", "lambda.model", "A.model", "A.orig.model", "dY.model",
   "dY.orig.model", "tD.linfit", "tD2.linfit", "tD.spline", "tD2.spline", "mu.spline",
    "lambda.spline", "A.spline", "dY.spline", "integral.spline", "mu2.spline",
   "lambda2.spline", "mu.bt", "lambda.bt", "A.bt", "integral.bt", "max_slope.linfit",
    "max_slope.spline"),
  pal = c("Green", "Orange", "Purple", "Magenta", "Grey", "Blue", "Grey", "Red", "Cyan",
    "Brown", "Mint"),
  invert.pal = FALSE,
  IDs = NULL,
  sort_by_ID = FALSE,
  names = NULL,
  conc = NULL,
  exclude.nm = NULL,
  exclude.conc = NULL,
  mean = TRUE,
  log.y = TRUE,
  n.ybreaks = 6,
  sort_by_conc = TRUE,
  nrow = NULL,
  basesize = 20,
  y.lim = NULL,
  x.lim = NULL,
  legend.lim = NULL,
  y.title = NULL,
  x.title = NULL,
  lwd = 1.1,
  plot = TRUE,
  export = FALSE,
  height = NULL,
  width = NULL,
  out.dir = NULL,
  out.nm = NULL,
```

```
  ...
)
```

Arguments

x	A grofit or flFitRes object created with growth.workflow or fl.workflow containing spline fits.
data.type	(Character) Plot either raw data (data.type = "raw") or the spline fit results
param	(Character) The parameter used to compare different sample groups. Any name of a column containing numeric values in gcTable (which is stored within grofit or gcFit objects) can be used as input. Useful options are: 'mu.linfit', 'lambda.linfit', 'dY.linfit', 'A.linfit', 'mu.model', 'lambda.model', 'A.model', 'mu.spline', 'lambda.spline', 'A.spline', 'dY.spline', 'integral.spline', 'mu.bt', 'lambda.bt', 'A.bt', 'integral.bt'
pal	(Character string) Choose one of 'Green', 'Orange', 'Purple', 'Magenta', 'Grey', 'Blue', 'Grey', 'Red', 'Cyan', 'Brown', or 'Mint' to visualize the value of the parameter chosen as param for each sample or condition.
invert.pal	(Logical) Shall the colors in the chosen pal be inverted (TRUE) or not FALSE?
IDs	(String or vector of strings) Define samples or groups (if mean = TRUE) to combine into a single plot based on exact matches with entries in the label or condition columns of grofit$expdesign. The order of strings within the vector defines the order of samples within the grid.
sort_by_ID	(Logical) Shall samples/conditions be ordered as entered in IDs (TRUE) or alphabetically (FALSE)?
names	(String or vector of strings) Define groups to combine into a single plot. Partial matches with sample/group names are accepted. If NULL, all samples are considered. Note: Ensure to use unique substrings to extract groups of interest. If the name of one condition is included in its entirety within the name of other conditions, it cannot be extracted individually.
conc	(Numeric or numeric vector) Define concentrations to combine into a single plot. If NULL, all concentrations are considered. Note: Ensure to use unique concentration values to extract groups of interest. If the concentration value of one condition is included in its entirety within the name of other conditions (e.g., the dataset contains '1', '10', and '100', code = 10 will select both '10 and '100'), it cannot be extracted individually.
exclude.nm	(String or vector of strings) Define groups to exclude from the plot. Partial matches with sample/group names are accepted.
exclude.conc	(Numeric or numeric vector) Define concentrations to exclude from the plot.
mean	(Logical) Display the mean and standard deviation of groups with replicates (TRUE) or plot each sample individually (FALSE)?
log.y	(Logical) Log-transform the y-axis of the plot (TRUE) or not (FALSE)?# '
n.ybreaks	(Numeric) Number of breaks on the y-axis. The breaks are generated using scales::pretty_breaks. Thus, the final number of breaks can deviate from the user input.

sort_by_conc	(Logical) Shall the samples/conditions be sorted with concentrations in rows and groups in columns?
nrow	(Numeric) Defines the number of rows in the grid if sort_by_conc is FALSE.
basesize	(Numeric) Base font size.
y.lim	(Numeric vector with two elements) Optional: Provide the lower (l) and upper (u) bounds of the y-axis of the growth curve plot as a vector in the form c(l, u). If only the lower or upper bound should be fixed, provide c(l, NA) or c(NA, u), respectively.
x.lim	(Numeric vector with two elements) Optional: Provide the lower (l) and upper (u) bounds of the x-axis of both growth curve and derivative plots as a vector in the form c(l, u). If only the lower or upper bound should be fixed, provide c(l, NA) or c(NA, u), respectively.
legend.lim	(Numeric vector with two elements) Optional: Provide the lower (l) and upper (u) bounds of the color scale applied to param as a vector in the form c(l, u). If only the lower or upper bound should be fixed, provide c(l, NA) or c(NA, u), respectively.
y.title	(Character) Optional: Provide a title for the y-axis of the growth curve plot.
x.title	(Character) Optional: Provide a title for the x-axis of both growth curve and derivative plots.
lwd	(Numeric) Line width of the individual plots.
plot	(Logical) Show the generated plot in the Plots pane (TRUE) or not (FALSE). If FALSE, a ggplot object is returned.
export	(Logical) Export the generated plot as PDF and PNG files (TRUE) or not (FALSE).
height	(Numeric) Height of the exported image in inches.
width	(Numeric) Width of the exported image in inches.
out.dir	(Character) Name or path to a folder in which the exported files are stored. If NULL, a "Plots" folder is created in the current working directory to store the files in.
out.nm	(Character) The name of the PDF and PNG files if export = TRUE. If NULL, a name will be automatically generated including the chosen parameter.
...	Additional arguments. This has currently no effect and is only meant to fulfill the requirements of a generic function.

Value

A plot matrix with all growth curves (raw measurements or nonparametric fits) in a dataset, with replicates combined by the group averages (if mean = TRUE) or not (mean = FALSE).

Examples

```
# Create random growth data set
rnd.data1 <- rdm.data(d = 35, mu = 0.8, A = 5, label = "Test1")
rnd.data2 <- rdm.data(d = 35, mu = 0.6, A = 4.5, label = "Test2")

rnd.data <- list()
```

```
rnd.data[["time"]] <- rbind(rnd.data1$time, rnd.data2$time)
rnd.data[["data"]] <- rbind(rnd.data1$data, rnd.data2$data)

# Run growth curve analysis workflow
res <- growth.workflow(time = rnd.data$time,
                       data = rnd.data$data,
                       fit.opt = "s",
                       ec50 = FALSE,
                       export.res = FALSE,
                       suppress.messages = TRUE,
                       parallelize = FALSE)


plot.grid(res, param = "mu.spline")
```

`plot.grodata` *Generic plot function for* `grodata` *objects. Plots raw growth, fluorescence, or normalized fluorescence data of multiple samples or conditions.*

Description

`plot.grodata` calls `plot.grofit` or `plot.flFitRes` based on the chosen `data.type`, respectively.

Usage

```
## S3 method for class 'grodata'
plot(
  x,
  data.type = c("growth", "fl", "norm.fl"),
  IDs = NULL,
  names = NULL,
  conc = NULL,
  mean = TRUE,
  exclude.nm = NULL,
  exclude.conc = NULL,
  log.y = FALSE,
  n.ybreaks = 6,
  colors = NULL,
  color_groups = TRUE,
 group_pals = c("Green", "Orange", "Purple", "Magenta", "Grey", "Blue", "Grey", "Red",
    "Cyan", "Brown", "Mint"),
  basesize = 20,
  y.lim = NULL,
  x.lim = NULL,
  y.title = NULL,
```

```
  x.title = NULL,
  lwd = 1.1,
  legend.position = "bottom",
  legend.ncol = 2,
  plot = TRUE,
  export = FALSE,
  height = NULL,
  width = NULL,
  out.dir = NULL,
  out.nm = NULL,
  ...
)
```

Arguments

x	A grodata object created with read_data or parse_data.
data.type	(Character) Plot either raw growth (data.type = "growth"), raw fluorescence (data.type = "fl"), or fluorescence normalized to growth (data.type = "norm.fl").
IDs	(String or vector of strings) Define samples or groups (if mean = TRUE) to combine into a single plot based on exact matches with entries in the label or condition columns of grofit$expdesign.
names	(String or vector of strings) Define groups to combine into a single plot. Partial matches with sample/group names are accepted. If NULL, all samples are considered. Note: Ensure to use unique substrings to extract groups of interest. If the name of one condition is included in its entirety within the name of other conditions, it cannot be extracted individually.
conc	(Numeric or numeric vector) Define concentrations to combine into a single plot. If NULL, all concentrations are considered. Note: Ensure to use unique concentration values to extract groups of interest. If the concentration value of one condition is included in its entirety within the name of other conditions (e.g., the dataset contains '1', '10', and '100', code = 10 will select both '10 and '100'), it cannot be extracted individually.
mean	(Logical) Display the mean and standard deviation of groups with replicates (TRUE) or plot each sample individually (FALSE)?
exclude.nm	(String or vector of strings) Define groups to exclude from the plot. Partial matches with sample/group names are accepted.
exclude.conc	(Numeric or numeric vector) Define concentrations to exclude from the plot.
log.y	(Logical) Log-transform the y-axis of the plot (TRUE) or not (FALSE)?
n.ybreaks	(Numeric) Number of breaks on the y-axis. The breaks are generated using scales::pretty_breaks. Thus, the final number of breaks can deviate from the user input.
colors	(vector of strings) Define a color palette used to draw the plots. If NULL, default palettes are chosen based on the number of groups/samples within the plot. Note: The number of provided colors should at least match the number of groups/samples.

color_groups (Logical) Shall samples within the same group but with different concentrations be shown in different shades of the same color?

group_pals (String vector) Define the colors used to display sample groups with identical concentrations. The number of selected color palettes must be at least the number of displayed groups. The order of the chosen palettes corresponds to the oder of conditions in the legend. Available options: "Green", "Oranges", "Purple", "Cyan", "Grey", "Red", "Blue", and "Magenta".

basesize (Numeric) Base font size.

y.lim (Numeric vector with two elements) Optional: Provide the lower (`l`) and upper (`u`) bounds of the y-axis of the growth curve plot as a vector in the form `c(l, u)`. If only the lower or upper bound should be fixed, provide `c(l, NA)` or `c(NA, u)`, respectively.

x.lim (Numeric vector with two elements) Optional: Provide the lower (`l`) and upper (`u`) bounds of the x-axis of both growth curve and derivative plots as a vector in the form `c(l, u)`. If only the lower or upper bound should be fixed, provide `c(l, NA)` or `c(NA, u)`, respectively.

y.title (Character) Optional: Provide a title for the y-axis of the growth curve plot.

x.title (Character) Optional: Provide a title for the x-axis of both growth curve and derivative plots.

lwd (Numeric) Line width of the individual plots.

legend.position (Character) Position of the legend. One of "bottom", "top", "left", "right".

legend.ncol (Numeric) Number of columns in the legend.

plot (Logical) Show the generated plot in the `Plots` pane (`TRUE`) or not (`FALSE`). If `FALSE`, a ggplot object is returned.

export (Logical) Export the generated plot as PDF and PNG files (`TRUE`) or not (`FALSE`).

height (Numeric) Height of the exported image in inches.

width (Numeric) Width of the exported image in inches.

out.dir (Character) Name or path to a folder in which the exported files are stored. If `NULL`, a "Plots" folder is created in the current working directory to store the files in.

out.nm (Character) The name of the PDF and PNG files if `export = TRUE`. If `NULL`, a name will be automatically generated including the chosen parameter.

... Additional arguments. This has currently no effect and is only meant to fulfill the requirements of a generic function.

Value

A plot with all growth curves (raw measurements) in a dataset, with replicates combined by the group averages (if `mean = TRUE`) or not (`mean = FALSE`).

Examples

```
# Create random growth data sets
rnd.data1 <- rdm.data(d = 35, mu = 0.8, A = 5, label = "Test1")
rnd.data2 <- rdm.data(d = 35, mu = 0.6, A = 4.5, label = "Test2")

# Create dataframe with both data sets and a single time vector
time <- as.data.frame(matrix(t(c("Time",NA,NA, rnd.data1$time[1,])),nrow=1),
            stringsAsFactors=FALSE)
colnames(time) <- colnames(rnd.data1$data)
data <- rbind(time, rnd.data1$data, rnd.data2$data)


# Create a grodata object
grodata <- read_data(data.growth = data, data.format = "row")

plot(grodata, exclude.nm = "Test1", legend.ncol = 4)
```

`plot.grofit` *Generic plot function for* `grofit` *objects. Combine different groups of samples into a single plot*

Description

`plot.grofit` extracts the spline fits of a subset of samples in a `grofit` object calculates averages and standard deviations of conditions with replicates and combines them into a single plot.

Usage

```
## S3 method for class 'grofit'
plot(
  x,
  ...,
  data.type = c("spline", "raw"),
  IDs = NULL,
  names = NULL,
  conc = NULL,
  exclude.nm = NULL,
  exclude.conc = NULL,
  mean = TRUE,
  log.y = TRUE,
  deriv = TRUE,
  n.ybreaks = 6,
  colors = NULL,
  color_groups = TRUE,
 group_pals = c("Green", "Orange", "Purple", "Magenta", "Grey", "Blue", "Grey", "Red",
    "Cyan", "Brown", "Mint"),
  basesize = 20,
```

```
  y.lim = NULL,
  x.lim = NULL,
  y.title = NULL,
  x.title = NULL,
  y.lim.deriv = NULL,
  y.title.deriv = NULL,
  lwd = 1.1,
  legend.position = "bottom",
  legend.ncol = 2,
  plot = TRUE,
  export = FALSE,
  height = NULL,
  width = NULL,
  out.dir = NULL,
  out.nm = NULL
)
```

Arguments

x	A grofit object created with growth.workflow containing spline fits.
...	(*optional*) Additional grofit objects created in separate workflows for joint plotting in a single graph.
data.type	(Character) Plot either raw data (data.type = "raw") or the spline fit results
IDs	(String or vector of strings) Define samples or groups (if mean = TRUE) to combine into a single plot based on exact matches with entries in the label or condition columns of grofit$expdesign.
names	(String or vector of strings) Define groups to combine into a single plot. Partial matches with sample/group names are accepted. If NULL, all samples are considered. Note: Ensure to use unique substrings to extract groups of interest. If the name of one condition is included in its entirety within the name of other conditions, it cannot be extracted individually.
conc	(Numeric or numeric vector) Define concentrations to combine into a single plot. If NULL, all concentrations are considered. Note: Ensure to use unique concentration values to extract groups of interest. If the concentration value of one condition is included in its entirety within the name of other conditions (e.g., the dataset contains '1', '10', and '100', code = 10 will select both '10 and '100'), it cannot be extracted individually.
exclude.nm	(String or vector of strings) Define groups to exclude from the plot. Partial matches with sample/group names are accepted.
exclude.conc	(Numeric or numeric vector) Define concentrations to exclude from the plot.
mean	(Logical) Display the mean and standard deviation of groups with replicates (TRUE) or plot each sample individually (FALSE)?
log.y	(Logical) Log-transform the y-axis of the plot (TRUE) or not (FALSE)?
deriv	(Logical) Show derivatives over time in a separate panel below the plot (TRUE) or not (FALSE)?

n.ybreaks	(Numeric) Number of breaks on the y-axis. The breaks are generated using scales::pretty_breaks. Thus, the final number of breaks can deviate from the user input.
colors	(vector of strings) Define a color palette used to draw the plots. If NULL, default palettes are chosen based on the number of groups/samples within the plot. Note: The number of provided colors should at least match the number of groups/samples.
color_groups	(Logical) Shall samples within the same group but with different concentrations be shown in different shades of the same color?
group_pals	(String vector) Define the colors used to display sample groups with identical concentrations. The number of selected color palettes must be at least the number of displayed groups. The order of the chosen palettes corresponds to the oder of conditions in the legend. Available options: "Green", "Oranges", "Purple", "Cyan", "Grey", "Red", "Blue", and "Magenta".
basesize	(Numeric) Base font size.
y.lim	(Numeric vector with two elements) Optional: Provide the lower (l) and upper (u) bounds of the y-axis of the growth curve plot as a vector in the form c(l, u). If only the lower or upper bound should be fixed, provide c(l, NA) or c(NA, u), respectively.
x.lim	(Numeric vector with two elements) Optional: Provide the lower (l) and upper (u) bounds of the x-axis of both growth curve and derivative plots as a vector in the form c(l, u). If only the lower or upper bound should be fixed, provide c(l, NA) or c(NA, u), respectively.
y.title	(Character) Optional: Provide a title for the y-axis of the growth curve plot.
x.title	(Character) Optional: Provide a title for the x-axis of both growth curve and derivative plots.
y.lim.deriv	(Numeric vector with two elements) Optional: Provide the lower (l) and upper (u) bounds on the y-axis of the derivative plot as a vector in the form c(l, u). If only the lower or upper bound should be fixed, provide c(l, NA) or c(NA, u), respectively.
y.title.deriv	(Character) Optional: Provide a title for the y-axis of the derivative plot.
lwd	(Numeric) Line width of the individual plots.
legend.position	(Character) Position of the legend. One of "bottom", "top", "left", "right".
legend.ncol	(Numeric) Number of columns in the legend.
plot	(Logical) Show the generated plot in the Plots pane (TRUE) or not (FALSE). If FALSE, a ggplot object is returned.
export	(Logical) Export the generated plot as PDF and PNG files (TRUE) or not (FALSE).
height	(Numeric) Height of the exported image in inches.
width	(Numeric) Width of the exported image in inches.
out.dir	(Character) Name or path to a folder in which the exported files are stored. If NULL, a "Plots" folder is created in the current working directory to store the files in.
out.nm	(Character) The name of the PDF and PNG files if export = TRUE. If NULL, a name will be automatically generated including the chosen parameter.

Value

A plot with all growth curves (raw measurements or nonparametric fits) in a dataset, with replicates combined by the group averages (if mean = TRUE) or not (mean = FALSE).

Examples

```
# Create random growth data set
rnd.data1 <- rdm.data(d = 35, mu = 0.8, A = 5, label = "Test1")
rnd.data2 <- rdm.data(d = 35, mu = 0.6, A = 4.5, label = "Test2")

rnd.data <- list()
rnd.data[["time"]] <- rbind(rnd.data1$time, rnd.data2$time)
rnd.data[["data"]] <- rbind(rnd.data1$data, rnd.data2$data)

# Run growth curve analysis workflow
res <- growth.workflow(time = rnd.data$time,
                       data = rnd.data$data,
                       fit.opt = "s",
                       ec50 = FALSE,
                       export.res = FALSE,
                       suppress.messages = TRUE,
                       parallelize = FALSE)


plot(res, names = "Test1", legend.ncol = 4) # Show only samples for condition "Test1"
```

---

plot.parameter *Compare growth parameters between samples or conditions*

Description

plot.parameter gathers physiological parameters from the results of a growth fit analysis and compares a chosen parameter between each sample or condition in a column plot. Error bars represent the 95% confidence interval (only shown for > 2 replicates).

Usage

```
## S3 method for class 'parameter'
plot(
  x,
  param = c("mu.linfit", "lambda.linfit", "dY.linfit", "A.linfit", "mu2.linfit",
   "lambda2.linfit", "mu.model", "lambda.model", "A.model", "A.orig.model", "dY.model",
   "dY.orig.model", "tD.linfit", "tD2.linfit", "tD.spline", "tD2.spline", "mu.spline",
     "lambda.spline", "A.spline", "dY.spline", "integral.spline", "mu2.spline",
   "lambda2.spline", "mu.bt", "lambda.bt", "A.bt", "integral.bt", "max_slope.linfit",
     "max_slope.spline"),
  IDs = NULL,
```

```
  names = NULL,
  conc = NULL,
  exclude.nm = NULL,
  exclude.conc = NULL,
  reference.nm = NULL,
  reference.conc = NULL,
  order_by_conc = FALSE,
  colors = NULL,
  basesize = 12,
  label.size = NULL,
  shape.size = 2.5,
  legend.position = "right",
  legend.ncol = 1,
  plot = TRUE,
  export = FALSE,
  height = 7,
  width = NULL,
  out.dir = NULL,
  out.nm = NULL,
  ...
)
```

Arguments

x	A grofit, gcFit, or gcTable object obtained with growth.workflow or growth.gcFit.
param	(Character) The parameter used to compare different sample groups. Any name of a column containing numeric values in gcTable (which is stored within grofit or gcFit objects) can be used as input. Useful options are: 'mu.linfit', 'lambda.linfit', 'dY.linfit', 'A.linfit', 'mu.model', 'lambda.model', 'A.model', 'mu.spline', 'lambda.spline', 'A.spline', 'dY.spline', 'integral.spline', 'mu.bt', 'lambda.bt', 'A.bt', 'integral.bt'
IDs	(String or vector of strings) Define samples or groups (if mean = TRUE) to combine into a single plot based on exact matches with entries in the label or condition columns of grofit$expdesign.
names	(String or vector of strings) Define groups to combine into a single plot. Partial matches with sample/group names are accepted. If NULL, all samples are considered. Note: Ensure to use unique substrings to extract groups of interest. If the name of one condition is included in its entirety within the name of other conditions, it cannot be extracted individually.
conc	(Numeric or numeric vector) Define concentrations to combine into a single plot. If NULL, all concentrations are considered. Note: Ensure to use unique concentration values to extract groups of interest. If the concentration value of one condition is included in its entirety within the name of other conditions (e.g., the dataset contains '1', '10', and '100', code = 10 will select both '10 and '100'), it cannot be extracted individually.
exclude.nm	(String or vector of strings) Define groups to exclude from the plot. Partial matches with sample/group names are accepted.

exclude.conc	(Numeric or numeric vector) Define concentrations to exclude from the plot.
reference.nm	(Character) Name of the reference condition, to which parameter values are normalized. Partially matching strings are tolerated as long as they can uniquely identify the condition.
reference.conc	(Numeric) Concentration of the reference condition, to which parameter values are normalized.
order_by_conc	(Logical) Shall the columns be sorted in order of ascending concentrations (TRUE) or by sample groups FALSE?
colors	(vector of strings) Define a color palette used to draw the columns. If NULL, default palettes are chosen. Note: The number of provided colors should at least match the number of groups.
basesize	(Numeric) Base font size.
label.size	(Numeric) Font size for sample labels below x-axis.
shape.size	(Numeric) The size of the symbols indicating replicate values. Default: 2.5
legend.position	(Character) Position of the legend. One of "bottom", "top", "left", "right".
legend.ncol	(Numeric) Number of columns in the legend.
plot	(Logical) Show the generated plot in the Plots pane (TRUE) or not (FALSE). If FALSE, a ggplot object is returned.
export	(Logical) Export the generated plot as PDF and PNG files (TRUE) or not (FALSE).
height	(Numeric) Height of the exported image in inches.
width	(Numeric) Width of the exported image in inches.
out.dir	(Character) Name or path to a folder in which the exported files are stored. If NULL, a "Plots" folder is created in the current working directory to store the files in.
out.nm	(Character) The name of the PDF and PNG files if export = TRUE. If NULL, a name will be automatically generated including the chosen parameter.
...	Additional arguments. This has currently no effect and is only meant to fulfill the requirements of a generic function.

Value

A column plot comparing a selected growth parameter between tested conditions.

Examples

```
# Create random growth data set
rnd.data1 <- rdm.data(d = 35, mu = 0.8, A = 5, label = "Test1")
rnd.data2 <- rdm.data(d = 35, mu = 0.6, A = 4.5, label = "Test2")

rnd.data <- list()
rnd.data[["time"]] <- rbind(rnd.data1$time, rnd.data2$time)
rnd.data[["data"]] <- rbind(rnd.data1$data, rnd.data2$data)

# Run growth curve analysis workflow
```

```
res <- growth.workflow(time = rnd.data$time,
                       data = rnd.data$data,
                       fit.opt = "s",
                       ec50 = FALSE,
                       export.res = FALSE,
                       parallelize = FALSE,
                       suppress.messages = TRUE)


plot.parameter(res,
               param = "mu.spline",
               legend.ncol = 4,
               legend.position = "bottom",
               basesize = 15,
               label.size = 11)
```

`rdm.data` *The function calls the* `baranyi` *function to generate curves between time zero and* `t` *and adds some random noise to the x- and y-axes. The three growth parameters given as input values will be slightly changed to produce different growth curves. The resulting datasets can be used to test the* `growth.workflow` *function.*

Description

The function calls the `baranyi` function to generate curves between time zero and `t` and adds some random noise to the x- and y-axes. The three growth parameters given as input values will be slightly changed to produce different growth curves. The resulting datasets can be used to test the `growth.workflow` function.

Usage

```
rdm.data(d, y0 = 0.05, tmax = 24, mu = 0.6, lambda = 5, A = 3, label = "Test1")
```

Arguments

`d`	Numeric value, number of data sets. If `d` is a vector, only the first entry is used.
`y0`	Numeric value, start growth. If `t` is a vector, only the first entry is used.
`tmax`	Numeric value, number of time points per data set. If `t` is a vector, only the first entry is used.
`mu`	Numeric value, maximum slope. If `mu` is a vector, only the first entry is used.
`lambda`	Numeric value, lag-phase. If `lambda` is a vector, only the first entry is used.
`A`	Numeric value, maximum growth. If `A` is a vector, only the first entry is used.
`label`	Character string, condition label If `label` is a vector, only the first entry is used.

Value

A list containing simulated data for three tests (e.g., 'organisms'):

`time`	numeric matrix of size `dxt`, each row represent the time points for which growth data is simulated and stored in each row of `data`.
`data`	data.frame of size dx(3+t), 1. column, character as an experiment identifier; 2. column: Replicate number; 3. column: concentration of substrate of a compound under which the experiment is obtained; 4.-(3+t). column: growth data corresponding to the time points in `time`.

References

Matthias Kahm, Guido Hasenbrink, Hella Lichtenberg-Frate, Jost Ludwig, Maik Kschischo (2010). *grofit: Fitting Biological Growth Curves with R*. Journal of Statistical Software, 33(7), 1-21. DOI: 10.18637/jss.v033.i07

Examples

```
# Create random growth data set
rnd.data1 <- rdm.data(d = 35, mu = 0.8, A = 5, label = 'Test1')
rnd.data2 <- rdm.data(d = 35, mu = 0.6, A = 4.5, label = 'Test2')

rnd.data <- list()
rnd.data[['time']] <- rbind(rnd.data1$time, rnd.data2$time)
rnd.data[['data']] <- rbind(rnd.data1$data, rnd.data2$data)

# Run growth curve analysis workflow
gcFit <- growth.gcFit(time = rnd.data$time,
                      data = rnd.data$data,
                      parallelize = FALSE,
                      control = growth.control(fit.opt = 's',
                                               suppress.messages = TRUE))


# Perform dose-response analysis
drFit <- growth.drFit(gcTable = gcFit$gcTable,
             control = growth.control(dr.parameter = 'mu.spline'))

# Inspect results
summary(drFit)
plot(drFit)
```

`read_data` *Read growth and fluorescence data in table format*

Description

read_data reads table files or R dataframe objects containing growth and fluorescence data and extracts datasets, sample and group information, performs blank correction, applies data transformation (calibration), and combines technical replicates.

Usage

```
read_data(
  data.growth = NA,
  data.fl = NA,
  data.fl2 = NA,
  data.format = "col",
  csvsep = ";",
  dec = ".",
  csvsep.fl = ";",
  dec.fl = ".",
  csvsep.fl2 = ";",
  dec.fl2 = ".",
  sheet.growth = 1,
  sheet.fl = 1,
  sheet.fl2 = 1,
  fl.normtype = c("growth", "fl2"),
  subtract.blank = TRUE,
  convert.time = NULL,
  calib.growth = NULL,
  calib.fl = NULL,
  calib.fl2 = NULL
)
```

Arguments

data.growth — An R dataframe object or a table file with extension '.xlsx', '.xls', '.csv', '.tsv', or '.txt' containing growth data. The data must be either in the 'QurvE custom layout' or in 'tidy' (long) format. The first three table rows in the 'custom QurvE layout' contain:

1. Sample description
2. Replicate number (*optional*: followed by a letter to indicate technical replicates)
3. Concentration value (*optional*)

Data in 'tidy' format requires the following column headers:

1. "Time": time values
2. "Description": sample description
3. "Replicate": replicate number (*optional*)
4. "Concentration": concentration value (*optional*)
5. "Values": growth values (e.g., optical density)

`data.fl` (optional) An R dataframe object or a table file with extension '.xlsx', '.xls', '.csv', '.tsv', or '.txt' containing fluorescence data. Table layout must mimic that of `data.growth`.

`data.fl2` (optional) An R dataframe object or a table file with extension '.xlsx', '.xls', '.csv', '.tsv', or '.txt' containing measurements from a second fluorescence channel (used only to normalize `fluorescence` data). Table layout must mimic that of `data.growth`.

`data.format` (Character) "col" for samples in columns, or "row" for samples in rows. Default: `"col"`

`csvsep` (Character) separator used in CSV file storing growth data (ignored for other file types). Default: `";"`

`dec` (Character) decimal separator used in CSV, TSV or TXT file storing growth data. Default: `"."`

`csvsep.fl, csvsep.fl2`
(Character) separator used in CSV file storing fluorescence data (ignored for other file types). Default: `";"`

`dec.fl, dec.fl2`
(Character) decimal separator used in CSV, TSV or TXT file storing fluorescence data. Default: `"."`

`sheet.growth, sheet.fl, sheet.fl2`
(Numeric or Character) Number or name of the sheet with the respective data type in XLS or XLSX files (*optional*).

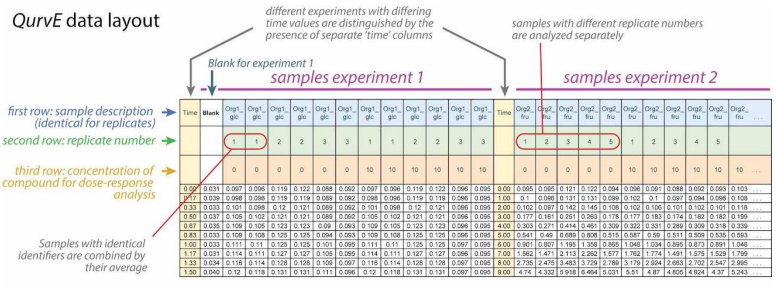
`fl.normtype` (Character string) Normalize fluorescence values by either diving by `'growth'` or by fluorescence2 values (`'fl2'`).

`subtract.blank` (Logical) Shall blank values be subtracted from values within the same experiment (TRUE, the default) or not (FALSE).

`convert.time` (NULL or string) Convert time values with a formula provided in the form `'y = function(x)'`. For example: `convert.time = 'y = 24 * x'`

`calib.growth, calib.fl, calib.fl2`
(Character or NULL) Provide an equation in the form 'y = function(x)' (for example: 'y = x^2 * 0.3 - 0.5') to convert growth and fluorescence values. This can be used to, e.g., convert plate reader absorbance values into OD_{600} or fluorescence intensity into molecule concentrations. Caution!: When utilizing calibration, carefully consider whether or not blanks were subtracted to determine the calibration before selecting the input `subtract.blank = TRUE`.

Details



Value

An R list object of class grodata containing a time matrix, dataframes with growth and fluorescence data (if applicable), and an experimental design table. The grodata object can be directly used to run growth.workflow/fl.workflow or, together with a growth.control/fl.control object, in growth.gcFit/flFit.

time	Matrix with raw time values extracted from data.growth.
growth	Dataframe with raw growth values and sample identifiers extracted from data.growth.
fluorescence	Dataframe with raw fluorescence values and sample identifiers extracted from data.fl. NA, if no fluorescence data is provided.
norm.fluorescence	fluorescence data divided by growth values. NA, if no fluorescence data is provided.
expdesign	Experimental design table created from the first three identifier rows/columns (see argument data.format) (data.growth.

Examples

```
# Load CSV file containing only growth data
data_growth <- read_data(data.growth = system.file("2-FMA_toxicity.csv",
                         package = "QurvE"), csvsep = ";" )

# Load XLS file containing both growth and fluorescence data
data_growth_fl <- read_data(
                 data.growth = system.file("lac_promoters_growth.txt", package = "QurvE"),
               data.fl = system.file("lac_promoters_fluorescence.txt", package = "QurvE"),
                    csvsep = "\t",
                    csvsep.fl = "\t")
```

---

read_file *Call the appropriate function required to read a table file and return the table as a dataframe object.*

Description

read_file automatically detects the format of a file provided as filename and calls the appropriate function to read the table file.

Usage

```
read_file(filename, csvsep = ";", dec = ".", sheet = 1)
```

Arguments

filename	(Character) Name or path of the table file to read. Can be of type CSV, XLS, XLSX, TSV, or TXT.
csvsep	(Character) separator used in CSV file (ignored for other file types).
dec	(Character) decimal separator used in CSV, TSV and TXT files.
sheet	(Numeric or Character) Number or name of a sheet in XLS or XLSX files (*optional*). Default: ";"

Value

A dataframe object with headers in the first row.

Examples

```
input <- read_file(filename = system.file("2-FMA_toxicity.csv", package = "QurvE"), csvsep = ";" )
```

---

run_app *Run Shiny QurvE App*

Description

Run Shiny QurvE App

Usage

```
run_app()
```

Value

Launches a browser with the shiny app

Examples

```
if(interactive()){
# Run the app
run_app()
}
```

summary.drBootSpline *Generic summary function for drBootSpline objects*

Description

Generic summary function for drBootSpline objects

Usage

```
## S3 method for class 'drBootSpline'
summary(object, ...)
```

Arguments

object	object of class drBootSpline
...	Additional arguments. This has currently no effect and is only meant to fulfill the requirements of a generic function.

Value

A dataframe with statistical parameters extracted from the dose-response bootstrapping analysis.

Examples

```
conc <- c(0, rev(unlist(lapply(1:18, function(x) 10*(2/3)^x))),10)
response <- c(1/(1+exp(-0.7*(4-conc[-20])))+stats::rnorm(19)/50, 0)

TestRun <- growth.drBootSpline(conc, response, drID = 'test',
        control = growth.control(log.x.dr = TRUE, smooth.dr = 0.8, nboot.dr = 50))

print(summary(TestRun))
```

summary.drFit *Generic summary function for drFit objects*

Description

Generic summary function for drFit objects

Usage

```
## S3 method for class 'drFit'
summary(object, ...)
```

Arguments

object	object of class drFit
...	Additional arguments. This has currently no effect and is only meant to fulfill the requirements of a generic function.

Value

A dataframe with parameters for all samples extracted from the dose-response analysis.

Examples

```
# Create random growth data set
rnd.data1 <- rdm.data(d = 35, mu = 0.8, A = 5, label = 'Test1')
rnd.data2 <- rdm.data(d = 35, mu = 0.6, A = 4.5, label = 'Test2')

rnd.data <- list()
rnd.data[['time']] <- rbind(rnd.data1$time, rnd.data2$time)
rnd.data[['data']] <- rbind(rnd.data1$data, rnd.data2$data)

# Run growth curve analysis workflow
gcFit <- growth.gcFit(time = rnd.data$time,
                      data = rnd.data$data,
                      parallelize = FALSE,
                      control = growth.control(fit.opt = 's',
                                               suppress.messages = TRUE))

# Perform dose-response analysis
drFit <- growth.drFit(gcTable = gcFit$gcTable,
                 control = growth.control(dr.parameter = 'mu.spline'))

# Inspect results
summary(drFit)
```

---

summary.drFitfl *Generic summary function for drFitfl objects*

Description

Generic summary function for drFitfl objects

Usage

```
## S3 method for class 'drFitfl'
summary(object, ...)
```

Arguments

object	object of class drFitfl
...	Additional arguments. This has currently no effect and is only meant to fulfill the requirements of a generic function.

Value

A dataframe with parameters for all samples extracted from a dose-response analysis.

Examples

```
# load example dataset
input <- read_data(data.growth = system.file("lac_promoters_growth.txt", package = "QurvE"),
              data.fl = system.file("lac_promoters_fluorescence.txt", package = "QurvE"),
                   csvsep = "\t",
                   csvsep.fl = "\t")

# Define fit controls
control <- fl.control(fit.opt = 's',
             x_type = 'time', norm_fl = TRUE,
             dr.parameter = 'max_slope.spline',
             dr.method = 'model',
             suppress.messages = TRUE)

# Run curve fitting workflow
res <- flFit(fl_data = input$norm.fluorescence,
             time = input$time,
             parallelize = FALSE,
             control = control)

# Perform dose-response analysis with biosensor model
drFitfl <- fl.drFit(flTable = res$flTable, control = control)

summary(drFitfl)
```

---

summary.drFitFLModel *Generic summary function for drFitFLModel objects*

Description

Generic summary function for drFitFLModel objects

Usage

```
## S3 method for class 'drFitFLModel'
summary(object, ...)
```

Arguments

object	object of class drFitModel
...	Additional arguments. This has currently no effect and is only meant to fulfill the requirements of a generic function.

Value

A dataframe with biosensor response parameters.

Examples

```
# Create concentration values via a serial dilution
conc <- c(0, rev(unlist(lapply(1:18, function(x) 10*(2/3)^x))),10)

# Simulate response values via biosensor equation
response <- biosensor.eq(conc, y.min = 110, y.max = 6000, K = 0.5, n = 2) +
            0.01*6000*rnorm(10)

# Perform fit
TestRun <- fl.drFitModel(conc, response, drID = 'test', control = fl.control())

print(summary(TestRun))
```

---

summary.drFitModel *Generic summary function for drFitModel objects*

Description

Generic summary function for drFitModel objects

Usage

```
## S3 method for class 'drFitModel'
summary(object, ...)
```

Arguments

object	object of class drFitModel
...	Additional arguments. This has currently no effect and is only meant to fulfill the requirements of a generic function.

Value

A dataframe with parameters extracted from the dose-response analysis of a single sample.

Examples

```
conc <- c(0, rev(unlist(lapply(1:18, function(x) 10*(2/3)^x))),10)
response <- c(1/(1+exp(-0.7*(4-conc[-20])))+rnorm(19)/50, 0)

TestRun <- growth.drFitModel(conc, response, drID = 'test')

print(summary(TestRun))
```

`summary.drFitSpline` *Generic summary function for drFitSpline objects*

Description

Generic summary function for drFitSpline objects

Usage

```
## S3 method for class 'drFitSpline'
summary(object, ...)
```

Arguments

`object`	object of class `drFitSpline`
`...`	Additional arguments. This has currently no effect and is only meant to fulfill the requirements of a generic function.

Value

A dataframe with parameters extracted from the dose-response analysis of a single sample.

Examples

```
conc <- c(0, rev(unlist(lapply(1:18, function(x) 10*(2/3)^x))),10)
response <- c(1/(1+exp(-0.7*(4-conc[-20])))+rnorm(19)/50, 0)

TestRun <- growth.drFitSpline(conc, response, drID = 'test',
              control = growth.control(log.x.dr = TRUE, smooth.dr = 0.8))

print(summary(TestRun))
```

summary.flBootSpline *Generic summary function for flBootSpline objects*

Description

Generic summary function for flBootSpline objects

Usage

```
## S3 method for class 'flBootSpline'
summary(object, ...)
```

Arguments

object	object of class flBootSpline
...	Additional arguments. This has currently no effect and is only meant to fulfill the requirements of a generic function.

Value

A dataframe with statistical parameters extracted from a dose-response bootstrapping analysis.

Examples

```
# load example dataset
input <- read_data(data.growth = system.file("lac_promoters_growth.txt", package = "QurvE"),
              data.fl = system.file("lac_promoters_fluorescence.txt", package = "QurvE"),
                   csvsep = "\t",
                   csvsep.fl = "\t")

# Extract time and normalized fluorescence data for single sample
time <- input$time[4,]
data <- input$norm.fluorescence[4,-(1:3)] # Remove identifier columns

# Perform linear fit
TestFit <- flBootSpline(time = time,
                        fl_data = data,
                        ID = 'TestFit',
                        control = fl.control(fit.opt = 's', x_type = 'time',
                        nboot.fl = 50))

summary(TestFit)
```

summary.flFit *Generic summary function for flFit objects*

Description

Generic summary function for flFit objects

Usage

```
## S3 method for class 'flFit'
summary(object, ...)
```

Arguments

object	object of class flFit
...	Additional arguments. This has currently no effect and is only meant to fulfill the requirements of a generic function.

Value

A dataframe with parameters extracted from all fits of a workflow.

Examples

```
# load example dataset
input <- read_data(data.growth = system.file("lac_promoters_growth.txt", package = "QurvE"),
              data.fl = system.file("lac_promoters_fluorescence.txt", package = "QurvE"),
                   csvsep = "\t",
                   csvsep.fl = "\t")

# Run curve fitting workflow
res <- flFit(fl_data = input$norm.fluorescence,
             time = input$time,
             parallelize = FALSE,
             control = fl.control(fit.opt = 's', suppress.messages = TRUE,
             x_type = 'time', norm_fl = TRUE, nboot.fl = 20))

summary(res)
```

summary.flFitLinear *Generic summary function for flFitLinear objects*

Description

Generic summary function for flFitLinear objects

Usage

```
## S3 method for class 'flFitLinear'
summary(object, ...)
```

Arguments

object	object of class flFitLinear
...	Additional arguments. This has currently no effect and is only meant to fulfill the requirements of a generic function.

Value

A dataframe with parameters extracted from a linear fit.

Examples

```
# load example dataset
input <- read_data(data.growth = system.file("lac_promoters_growth.txt", package = "QurvE"),
              data.fl = system.file("lac_promoters_fluorescence.txt", package = "QurvE"),
                   csvsep = "\t",
                   csvsep.fl = "\t")

# Extract time and normalized fluorescence data for single sample
time <- input$time[4,]
data <- input$norm.fluorescence[4,-(1:3)] # Remove identifier columns

# Perform linear fit
TestFit <- flFitLinear(time = time,
                       fl_data = data,
                       ID = 'TestFit',
                       control = fl.control(fit.opt = 'l', x_type = 'time',
                       lin.R2 = 0.95, lin.RSD = 0.1,
                       lin.h = 20))

summary(TestFit)
```

`summary.flFitSpline` *Generic summary function for flFitSpline objects*

Description

Generic summary function for flFitSpline objects

Usage

```
## S3 method for class 'flFitSpline'
summary(object, ...)
```

Arguments

`object`	object of class `flFitSpline`
`...`	Additional arguments. This has currently no effect and is only meant to fulfill the requirements of a generic function.

Value

A dataframe with parameters extracted from a nonparametric fit.

Examples

```
# load example dataset
input <- read_data(data.growth = system.file("lac_promoters_growth.txt", package = "QurvE"),
              data.fl = system.file("lac_promoters_fluorescence.txt", package = "QurvE"),
                   csvsep = "\t",
                   csvsep.fl = "\t")

# Extract time and normalized fluorescence data for single sample
time <- input$time[4,]
data <- input$norm.fluorescence[4,-(1:3)] # Remove identifier columns

# Perform linear fit
TestFit <- flFitSpline(time = time,
                       fl_data = data,
                       ID = 'TestFit',
                       control = fl.control(fit.opt = 's', x_type = 'time'))

summary(TestFit)
```

summary.gcBootSpline *Generic summary function for gcBootSpline objects*

Description

Generic summary function for gcBootSpline objects

Usage

```
## S3 method for class 'gcBootSpline'
summary(object, ...)
```

Arguments

object	object of class gcBootSpline
...	Additional arguments. This has currently no effect and is only meant to fulfill the requirements of a generic function.

Value

A dataframe with statistical parameters extracted from the spline fit bootstrapping computation.

Examples

```
# Create random growth dataset
rnd.dataset <- rdm.data(d = 35, mu = 0.8, A = 5, label = 'Test1')

# Extract time and growth data for single sample
time <- rnd.dataset$time[1,]
data <- rnd.dataset$data[1,-(1:3)] # Remove identifier columns

# Introduce some noise into the measurements
data <- data + stats::runif(97, -0.01, 0.09)

# Perform bootstrapping spline fit
TestFit <- growth.gcBootSpline(time, data, gcID = 'TestFit',
              control = growth.control(fit.opt = 's', nboot.gc = 50))

summary(TestFit)
```

`summary.gcFit` *Generic summary function for gcFit objects*

Description

Generic summary function for gcFit objects

Usage

```
## S3 method for class 'gcFit'
summary(object, ...)
```

Arguments

`object`	object of class `gcFit`
`...`	Additional arguments. This has currently no effect and is only meant to fulfill the requirements of a generic function.

Value

A dataframe with parameters extracted from all fits of a workflow.

Examples

```
# Create random growth data set
rnd.data1 <- rdm.data(d = 35, mu = 0.8, A = 5, label = 'Test1')
rnd.data2 <- rdm.data(d = 35, mu = 0.6, A = 4.5, label = 'Test2')

rnd.data <- list()
rnd.data[['time']] <- rbind(rnd.data1$time, rnd.data2$time)
rnd.data[['data']] <- rbind(rnd.data1$data, rnd.data2$data)

# Run growth curve analysis workflow
gcFit <- growth.gcFit(time = rnd.data$time,
                      data = rnd.data$data,
                      parallelize = FALSE,
                      control = growth.control(fit.opt = 's',
                                               suppress.messages = TRUE,
                                               nboot.gc = 20))
summary(gcFit)
```

summary.gcFitLinear *Generic summary function for gcFitLinear objects*

Description

Generic summary function for gcFitLinear objects

Usage

```
## S3 method for class 'gcFitLinear'
summary(object, ...)
```

Arguments

object	object of class gcFitLinear
...	Additional arguments. This has currently no effect and is only meant to fulfill the requirements of a generic function.

Value

A dataframe with parameters extracted from the linear fit.

Examples

```
# Create random growth dataset
rnd.dataset <- rdm.data(d = 35, mu = 0.8, A = 5, label = 'Test1')

# Extract time and growth data for single sample
time <- rnd.dataset$time[1,]
data <- rnd.dataset$data[1,-(1:3)] # Remove identifier columns

# Perform linear fit
TestFit <- growth.gcFitLinear(time, data, gcID = 'TestFit',
                 control = growth.control(fit.opt = 'l'))

summary(TestFit)
```

summary.gcFitModel *Generic summary function for gcFitModel objects*

Description

Generic summary function for gcFitModel objects

Usage

```
## S3 method for class 'gcFitModel'
summary(object, ...)
```

Arguments

object	object of class gcFitModel
...	Additional arguments. This has currently no effect and is only meant to fulfill the requirements of a generic function.

Value

A dataframe with parameters extracted from the growth model fit.

Examples

```
# Create random growth dataset
rnd.dataset <- rdm.data(d = 35, mu = 0.8, A = 5, label = 'Test1')

# Extract time and growth data for single sample
time <- rnd.dataset$time[1,]
data <- rnd.dataset$data[1,-(1:3)] # Remove identifier columns

# Perform parametric fit
TestFit <- growth.gcFitModel(time, data, gcID = 'TestFit',
                 control = growth.control(fit.opt = 'm'))

summary(TestFit)
```

---

summary.gcFitSpline *Generic summary function for gcFitSpline objects*

Description

Generic summary function for gcFitSpline objects

Usage

```
## S3 method for class 'gcFitSpline'
summary(object, ...)
```

Arguments

object	object of class gcFitSpline
...	Additional arguments. This has currently no effect and is only meant to fulfill the requirements of a generic function.

Value

A dataframe with parameters extracted from the nonparametric fit.

Examples

```
# Create random growth dataset
rnd.dataset <- rdm.data(d = 35, mu = 0.8, A = 5, label = 'Test1')

# Extract time and growth data for single sample
time <- rnd.dataset$time[1,]
data <- rnd.dataset$data[1,-(1:3)] # Remove identifier columns

# Perform linear fit
TestFit <- growth.gcFitSpline(time, data, gcID = 'TestFit',
                 control = growth.control(fit.opt = 's'))

summary(TestFit)
```

---

table_group_fluorescence_linear

Generate a grouped results table for linear fits with average and standard deviations

---

Description

Generate a grouped results table for linear fits with average and standard deviations

Usage

```
table_group_fluorescence_linear(flTable, html = FALSE)
```

Arguments

`flTable`	An object of class `flTable`
`html`	(Logical) Should column headers contain html formatting?

Value

A data frame with grouped linear fit results. Empty cells indicate that no reliable fit could be determined.

Examples

```
# load example dataset
input <- read_data(data.growth = system.file("lac_promoters_growth.txt", package = "QurvE"),
              data.fl = system.file("lac_promoters_fluorescence.txt", package = "QurvE"),
                   csvsep = "\t",
                   csvsep.fl = "\t")

# Run workflow
res <- fl.workflow(grodata = input, ec50 = FALSE, fit.opt = "l",
                   x_type = "time", norm_fl = TRUE,
                   dr.parameter = "max_slope.spline",
                   suppress.messages = TRUE,
                   parallelize = FALSE)

table_group_fluorescence_linear(res$flFit$flTable)

# with HTML formatting
DT::datatable(table_group_fluorescence_linear(res$flFit$flTable, html = TRUE),
              escape = FALSE) # Do not escape HTML entities
```

---

table_group_fluorescence_spline

Generate a grouped results table for spline fits with average and standard deviations

---

Description

Generate a grouped results table for spline fits with average and standard deviations

Usage

```
table_group_fluorescence_spline(flTable, html = FALSE)
```

Arguments

`flTable`	An object of class `flTable`
`html`	(Logical) Should column headers contain html formatting?

Value

A data frame with grouped spline fit results. Empty cells indicate that no reliable fit could be determined.

Examples

```
# load example dataset
input <- read_data(data.growth = system.file("lac_promoters_growth.txt", package = "QurvE"),
              data.fl = system.file("lac_promoters_fluorescence.txt", package = "QurvE"),
                   csvsep = "\t",
                   csvsep.fl = "\t")

# Run workflow
res <- fl.workflow(grodata = input, ec50 = FALSE, fit.opt = "s",
                   x_type = "time", norm_fl = TRUE,
                   dr.parameter = "max_slope.spline",
                   suppress.messages = TRUE,
                   parallelize = FALSE)

table_group_fluorescence_spline(res$flFit$flTable)

# with HTML formatting
DT::datatable(table_group_fluorescence_spline(res$flFit$flTable, html = TRUE),
              escape = FALSE) # Do not escape HTML entities
```

---

table_group_growth_linear

Generate a grouped results table for linear fits with average and standard deviations

---

Description

Generate a grouped results table for linear fits with average and standard deviations

Usage

```
table_group_growth_linear(gcTable, html = FALSE)
```

Arguments

gcTable	An object of class gcTable
html	(Logical) Should column headers contain html formatting?

Value

A data frame with grouped linear fit results. Empty cells indicate that no reliable fit could be determined.

Examples

```
# Create random growth data set
rnd.data <- rdm.data(d = 30, mu = 0.6, A = 4.5, label = "Test2")


# Run growth curve analysis workflow
res <- growth.workflow(time = rnd.data$time,
                       data = rnd.data$data,
                       fit.opt = "l",
                       ec50 = FALSE,
                       export.res = FALSE,
                       parallelize = FALSE,
                       suppress.messages = TRUE)

table_group_growth_linear(res$gcFit$gcTable)

# with HTML formatting
DT::datatable(table_group_growth_linear(res$gcFit$gcTable, html = TRUE),
              escape = FALSE) # Do not escape HTML entities
```

---

table_group_growth_model

Generate a grouped results table for parametric fits with average and standard deviations

---

Description

Generate a grouped results table for parametric fits with average and standard deviations

Usage

```
table_group_growth_model(gcTable, html = FALSE)
```

Arguments

gcTable	An object of class gcTable
html	(Logical) Should column headers contain html formatting?

Value

A data frame with grouped model fit results. Empty cells indicate that no reliable fit could be determined.

Examples

```
# Create random growth data set
rnd.data <- rdm.data(d = 35, mu = 0.8, A = 5, label = "Test1")


# Run growth curve analysis workflow
res <- growth.workflow(time = rnd.data$time,
                       data = rnd.data$data,
                       fit.opt = "m",
                       ec50 = FALSE,
                       export.res = FALSE,
                       parallelize = FALSE,
                       suppress.messages = TRUE)

table_group_growth_model(res$gcFit$gcTable)

# with HTML formatting
DT::datatable(table_group_growth_model(res$gcFit$gcTable, html = TRUE),
              escape = FALSE) # Do not escape HTML entities
```

---

table_group_growth_spline

Generate a grouped results table for spline fits with average and standard deviations

---

Description

Generate a grouped results table for spline fits with average and standard deviations

Usage

```
table_group_growth_spline(gcTable, html = FALSE)
```

Arguments

gcTable	An object of class gcTable
html	(Logical) Should column headers contain html formatting?

Value

A data frame with grouped spline fit results. Empty cells indicate that no reliable fit could be determined.

Examples

```
# Create random growth data set
rnd.data <- rdm.data(d = 35, mu = 0.8, A = 5, label = "Test1")

# Run growth curve analysis workflow
res <- growth.workflow(time = rnd.data$time,
                       data = rnd.data$data,
                       fit.opt = "s",
                       ec50 = FALSE,
                       export.res = FALSE,
                       parallelize = FALSE,
                       suppress.messages = TRUE)

table_group_growth_spline(res$gcFit$gcTable)

# with HTML formatting
DT::datatable(table_group_growth_spline(res$gcFit$gcTable, html = TRUE),
              escape = FALSE) # Do not escape HTML entities
```

---

zipFastener *Combine two dataframes like a zip-fastener*

Description

Combine rows or columns of two dataframes in an alternating manner

Usage

```
zipFastener(df1, df2, along = 2)
```

Arguments

df1	A first dataframe.
df2	A second dataframe with the same dimensions as df1.
along	1 to alternate rows or 2 to alternate columns.

Value

A dataframe with combined rows (or columns) of df1 and df2.

Author(s)

Mark Heckmann

Examples

```
# data frames equal dimensions
df1 <- plyr::rdply(3, rep('o',4))[ ,-1]
df2 <- plyr::rdply(3, rep('X',4))[ ,-1]

zipFastener(df1, df2)
zipFastener(df1, df2, 2)
zipFastener(df1, df2, 1)

# data frames unequal in no. of rows
df1 <- plyr::rdply(10, rep('o',4))[ ,-1]
zipFastener(df1, df2, 1)
zipFastener(df2, df1, 1)

# data frames unequal in no. of columns
df2 <- plyr::rdply(10, rep('X',3))[ ,-1]
zipFastener(df1, df2)
zipFastener(df2, df1, 2)
```

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