

Package ‘CalibraCurve’

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Title Calibration curves for targeted proteomics, lipidomics and metabolomics data

Version 1.2.0

Description CalibraCurve is a computational tool designed to generate calibration curves for targeted mass spectrometry-based quantitative data. It is applicable to various omics disciplines, including proteomics, lipidomics, and metabolomics. The package also offers functionalities for data and calibration curve visualization and concentration prediction from new datasets based on the established curves.

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.calcContPrelimRanges *PLR: Calculate key features for the existing continuous preliminary ranges*

Description

PLR: Calculate key features for the existing continuous preliminary ranges

Usage

```
.calcContPrelimRanges(index)
```

Arguments

index	integer
	Integer vector containing indices of concentration levels with CV < threshold.

Value

Data.frame with one range in each row. Contains the columns "startPoints", "endPoints", and "extent".

.calcCV *PLR: calculate CV for one concentration level*

Description

PLR: calculate CV for one concentration level

Usage

```
.calcCV(x)
```

Arguments

x	data.frame
	Data.frame containing data for a specific concentration level.

Value

numeric(1)
Coefficient of variation (CV) for the given concentration level.

<code>.calcLinearModel</code>	<i>FLR: calculate weighted or unweighted linear model</i>
-------------------------------	---

Description

FLR: calculate weighted or unweighted linear model

Usage

```
.calcLinearModel(x, weights = NULL)
```

Arguments

<code>x</code>	list of data.frames List of data frames (one entry for each concentration level), e.g. output "dataPrelim" from calculate_PLR .
<code>weights</code>	numeric Vector of weights as calculated by applying .calcWeights (default is NULL and will result in an unweighted model).

Value

Fit of the linear model as an object of class "lm".

<code>.calcPerBias</code>	<i>FLR: calculate percent bias for a specific concentration level</i>
---------------------------	---

Description

FLR: calculate percent bias for a specific concentration level

Usage

```
.calcPerBias(x, LMfit, expConc)
```

Arguments

<code>x</code>	data.frame Data.frame containing data for a specific concentration level.
<code>LMfit</code>	lm object Linear model fit as calculated by .calcLinearModel .
<code>expConc</code>	numeric(1) Expected (known) concentration level.

Value

Vector of percent bias values for each data point in this concentration level.

<code>.calcPerBiasAvgSDCV</code>	<i>FLR: calculate average, SD and CV percent bias for each concentration level</i>
----------------------------------	--

Description

FLR: calculate average, SD and CV percent bias for each concentration level

Usage

```
.calcPerBiasAvgSDCV(x, method = "mean")
```

Arguments

x	list Result of .calcPerBiasLevels .
method	character(1) Method for calculating the average percent bias: "mean" (default) or "median".

Value

data frame with 3 columns: avgPerBias, stdDevPerBias, CV_PerBias
each row is one concentration level

<code>.calcPerBiasLevels</code>	<i>FLR: calculate list of percent bias values for all concentration levels</i>
---------------------------------	--

Description

FLR: calculate list of percent bias values for all concentration levels

Usage

```
.calcPerBiasLevels(x, LMfit)
```

Arguments

x	list of data.frames List of data frames (one entry for each concentration level), e.g. output "dataPrelim" from calculate_PLR .
LMfit	lm object Linear model fit as calculated by .calcLinearModel .

Value

List with percent bias values for each data point per concentration level

`.calcResponseFactors` *Calculate Response factors*

Description

Function, which calculates a response factor for a single data point

Usage

```
.calcResponseFactors(x, intercept, expConc)
```

Arguments

<code>x</code>	<i>data.frame*</i> Data.frame containing data for a specific concentration level.
<code>intercept</code>	numeric(1) Intercept of the linear model.
<code>expConc</code>	numeric(1) Expected concentration (known concentration value).

Details

Formula obtained from: Green, J. M., A practical guide to analytical method validation. Analytical Chemistry 1996, 68, 305A-309A.

Value

vector of response factors for this specific concentration level

`.calcWeights` *FLR: calculate weights for linear model for a specific concentration level*

Description

FLR: calculate weights for linear model for a specific concentration level

Usage

```
.calcWeights(x, weightingMethod = "1/x^2")
```

Arguments

x	data.frame Data.frame containing data for a specific concentration level.
weightingMethod	character(1) Method for weighting (currently "1/x", "1/x^2" and "None" are supported, default is "1/x^2").

Value

Vector of a constant weights for each measurement in this concentration level.

.checkFinalRange	<i>FLR: checks if final linear range has been reached (compare average percent bias with threshold)</i>
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Description

FLR: checks if final linear range has been reached (compare average percent bias with threshold)

Usage

```
.checkFinalRange(perBiasInfo, perBiasThres = 20)
```

Arguments

perBiasInfo	data.frame Result of .calcPerBiasAvgSDCV .
perBiasThres	numeric(1) numeric(1) Threshold for average percent bias in percent, default is 20.

Value

TRUE if both lowest and highest concentration level passed the check (and the final linear range is reached), FALSE otherwise

`.checkNumberReplicates`

Data preprocessing: Helper function to check for sufficient number of replicates for a specific concentration level

Description

Data preprocessing: Helper function to check for sufficient number of replicates for a specific concentration level

Usage

```
.checkNumberReplicates(x, data, minReplicates)
```

Arguments

<code>x</code>	numeric(1) concentration level to check
<code>data</code>	list of data.frames list of data.frames (each dataframe contains data for a specific concentration level)
<code>minReplicates</code>	integer(1) minimal number of data points per concentration level

Value

logical(1)
TRUE if there are enough replicates, else FALSE

`.filterConcentrationLevel`

Data preprocessing: Helper function to select all rows from a specific concentration level

Description

Data preprocessing: Helper function to select all rows from a specific concentration level

Usage

```
.filterConcentrationLevel(x, data)
```

Arguments

<code>x</code>	numeric(1) concentration level to select
<code>data</code>	data.frame data set to be filtered (e.g., result of readDataTable)

Value

data.frame

<code>.prepareAnnotationData</code>	<i>Prepare annotation data</i>
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Description

Prepare annotation data

Usage

```
.prepareAnnotationData(D_calib)
```

Arguments

<code>D_calib</code>	data.frame Result of .prepareCalibData
----------------------	--

Value

Dataframe with annotation data for the plot.

<code>.prepareCalibData</code>	<i>Prepare calibration data</i>
--------------------------------	---------------------------------

Description

Prepare calibration data

Usage

```
.prepareCalibData(CC_RES)
```

Arguments

<code>CC_RES</code>	list Result object of CalibraCurve .
---------------------	---

Value

Dataframe with calibration data for plotting.

<code>.prepareCurveData</code>	<i>Prepare curve data</i>
--------------------------------	---------------------------

Description

Prepare curve data

Usage

```
.prepareCurveData(CC_RES, D_calib)
```

Arguments

<code>CC_RES</code>	list Results of CalibraCurve . Each list element is the result of calc_single_curve
<code>D_calib</code>	data.frame Result of .prepareCalibData

Value

Dataframe with data points on a grid to plot the calibration curve.

<code>.saveCCResult</code>	<i>Save results of CalibraCurve</i>
----------------------------	-------------------------------------

Description

Save results of CalibraCurve

Usage

```
.saveCCResult(CC_res, output_path, suffix = "")
```

Arguments

<code>CC_res</code>	list Result object of CalibraCurve .
<code>output_path</code>	character(1) Path to the output directory.
<code>suffix</code>	character(1) Suffix for the output files, ideally starting with "_" (default is "").

Value

Returns nothing, but the function saves the results to the specified output path.

.saveTablesAndPlots *Save result tables and plots*

Description

Save result tables and plots

Usage

```
.saveTablesAndPlots(  
  RES,  
  output_path,  
  pl_CC_list,  
  pl_RF_list,  
  summary_tab,  
  CC_plot_width,  
  CC_plot_height,  
  RF_plot_width,  
  RF_plot_height,  
  plot_type,  
  plot_dpi,  
  device  
)
```

Arguments

RES	list Results of CalibraCurve . Each list element is the result of calc_single_curve
output_path	character(1) Folder to save results (table and plots). If NULL (default), results are not saved.
pl_CC_list	list List of calibration curves (ggplot objects, results of plotCalibraCurve (CC_plot)).
pl_RF_list	list List of response factor plots (ggplot objects, results of plotResponseFactors).
summary_tab	data.frame Table with summary information, result of plotCalibraCurve (annotation_dat)
CC_plot_width	numeric(1) Plot width in cm (default is 10).
CC_plot_height	numeric(1) Plot height in cm (default is 10).
RF_plot_width	numeric(1) Plot width in cm (default is 10).
RF_plot_height	numeric(1) Plot height in cm (default is 10).

<code>plot_type</code>	character(1) Type of plot for calibration curves: "single_plots" (default, generate a separate plot for each substance), "multiplot" (generate a graphic with subplots for each substance) or "all_in_one" (generate a single plot with all substances).
<code>plot_dpi</code>	numeric(1) Plot resolution in dpi (default is 300).
<code>device</code>	character(1) Device for saving the plot (default is "png"). Other options include "pdf", "jpeg", "tiff", "svg" etc. For details see ggsave .

Value

Invisible NULL. Plots and the summary table are saved to the hard drive.

<code>.selctConcLevel</code>	<i>FLR: selects the highest or lowest concentration level for removal</i>
------------------------------	---

Description

FLR: selects the highest or lowest concentration level for removal

Usage

```
.selctConcLevel(x, perBiasT = 20, consPerBiasCV = TRUE, perBiasDistT = 10)
```

Arguments

<code>x</code>	data.frame Result of .calcPerBiasAvgSDCV .
<code>perBiasT</code>	numeric(1) Threshold for average percent bias in percent, default is 20.
<code>consPerBiasCV</code>	consider CV? default is TRUE
<code>perBiasDistT</code>	numeric(1) Threshold for the difference in average percent bias in percent (for lower differences, CV will be considered), default is 10. Only used if <code>consPerBiasCV</code> is TRUE.

Value

TRUE, if lowest concentration will be removed, FALSE if highest will be removed

assemble_results	<i>Assemble result tables</i>
------------------	-------------------------------

Description

Assemble result tables

Usage

```
assemble_results(
  X,
  dataCleaned,
  PLR_res,
  resFacDataV,
  avgResFacDataV,
  FLR_res,
  mod,
  cvThres = 20,
  RfThresL = 80,
  RfThresU = 120,
  substance = "substance1"
)
```

Arguments

X	data.frame Original data set, e.g. result of readDataTable .
dataCleaned	list of data.frames Cleaned data, result of cleanData .
PLR_res	list Result object of calculate_PLR .
resFacDataV	list List of response factor values for each concentration level.
avgResFacDataV	numeric Vector of mean response factor values for the different concentration levels.
FLR_res	list Result object of calculate_FLR .
mod	lm object Final linear model fit (object "mod" from results of calculate_FLR).
cvThres	numeric(1) Threshold for CV per concentration level in percent (default is 20).
RfThresL	numeric(1) Lower threshold for response factor in percent (default is 80).
RfThresU	numeric(1) Upper threshold for response factor in percent (default is 120).
substance	character(1) Name of the substance (default is "substance1").

Value

List with the following elements:

- `result_table_conc_levels`: Result table with one line for each concentration level.
- `result_table_obs`: Result table with one line per observation (e.g. individual response factors for each data point).

Examples

```
file <- system.file("extdata", "MSQC1", "msqc1_dil_GGPFSDSYR.rds",
  package = "CalibraCurve")
D_list <- readDataSE(file, concColName = "amount_fmol",
  substColName = "Substance", assayNumber = 1)
data_cleaned <- cleanData(D_list[[1]])

RES_PLR <- calculate_PLR(data_cleaned, calcContinuousPrelimRanges = FALSE)
RES_FLR <- calculate_FLR(RES_PLR$dataPrelim)
RFs <- calcRF(data_cleaned, mod = RES_FLR$mod)

assemble_results(
  X = D_list[[1]],
  dataCleaned = data_cleaned,
  PLR_res = RES_PLR,
  resFacDataV = RFs$RFs,
  avgResFacDataV = RFs$meanRFs,
  FLR_res = RES_FLR,
  mod = RES_FLR$mod
)
```

calcRF

Calculate Response factors

Description

Final linear range: Function, which returns a list with response factor values for a data set (given as list)

Usage

```
calcRF(x, mod)
```

Arguments

<code>x</code>	list of data.frames List of data.frames containing data for each concentration level (result from cleanData).
<code>mod</code>	lm object Final linear model fit (object "mod" from results of calculate_FLR).

Value

- List with the following elements:
- RFs: List with response factors for each concentration level.
 - meanRFs: Vector with mean response factors for each concentration level.
- response factor values for each concentration level.

Examples

```
file <- system.file("extdata", "MSQC1", "msqc1_dil_GGPFSDSYR.rds",
package = "CalibraCurve")
D_list <- readDataSE(file, concColName = "amount_fm1",
  substColName = "Substance", assayNumber = 1)
data_cleaned <- cleanData(D_list[[1]])
RES_PLR <- calculate_PLR(data_cleaned, calcContinuousPrelimRanges = FALSE)
RES_FLR <- calculate_FLR(RES_PLR$dataPrelim)

calcRF(data_cleaned, mod = RES_FLR$mod)
```

calculate_FLR	<i>Calculate the final linear range</i>
---------------	---

Description

Calculate the final linear range

Usage

```
calculate_FLR(
  dataPrelim,
  weightingMethod = "1/x^2",
  centralTendencyMeasure = "mean",
  perBiasThres = 20,
  considerPerBiasCV = TRUE,
  perBiasDistThres = 10
)
```

Arguments

- | | |
|-----------------|--|
| dataPrelim | list of data.frames
List of data.frames containing data only within the preliminary linear range (result from calculate_PLR). |
| weightingMethod | character(1)
Method for weighting (currently "1/x", "1/x^2" and "None" are supported, default is 1/x^2). |

centralTendencyMeasure
character(1)
 Method for calculating average percent bias, "mean" (default) or "median".

perBiasThres **numeric(1)**
 Threshold for average percent bias in percent, default is 20.

considerPerBiasCV
logical(1)
 If TRUE, CV is considered for the elimination of the concentration level (default). CV will only be considered if the difference in percent bias values is lower than perBiasDistThres.

perBiasDistThres
numeric(1)
 Threshold for the difference in average percent bias in percent (for lower differences, CV will be considered), default is 10. Only relevant if considerPerBiasCV = TRUE.

Value

List with the following elements:

- dataFinal: List of data.frames containing data only within the final linear range.
- mod: lm-object containing the final linear model (weighted or unweighted, depending on weightingMethod).
- perBias: result list of [.calcPerBiasLevels](#).
- perBiasAvgSDCV: result data.frame of [.calcPerBiasAvgSDCV](#).

Examples

```
file <- system.file("extdata", "MSQC1", "msqc1_dil_GGPFSDSYR.rds",
  package = "CalibraCurve")
D_list <- readDataSE(file, concColName = "amount_fm1",
  substColName = "Substance", assayNumber = 1)
data_cleaned <- cleanData(D_list[[1]])
RES_PLR <- calculate_PLR(data_cleaned, calcContinuousPrelimRanges = FALSE)

calculate_FLR(RES_PLR$dataPrelim)
```

calculate_PLR	<i>Calculate preliminary linear range (PLR)</i>
---------------	---

Description

Calculate preliminary linear range (PLR)

Usage

```
calculate_PLR(dataCleaned, cvThres = 20, calcContinuousPrelimRanges = TRUE)
```

Arguments

- dataCleaned** **data.frame**
Data cleaned by [cleanData](#).
- cvThres** **numeric(1)**
Threshold for CV per concentration level in percent (default is 20).
- calcContinuousPrelimRanges**
logical(1)
If TRUE, the longest continuous range fulfilling the CV threshold is selected (default is TRUE). If FALSE, gaps with CVs larger than the threshold may be included.

Value

List with the following elements:

- **dataPrelim**: List of data.frames containing data only within the preliminary linear range.
- **concLevelsCV**: Vector with the calculated CV for each concentration level.
- **prelimConcLevels**: Vector with the concentration levels within the preliminary linear range.

Examples

```
file <- system.file("extdata", "MSQC1", "msqc1_dil_GGPFSDSYR.rds",
  package = "CalibraCurve")
D_list <- readDataSE(file, concColName = "amount_fm1",
  substColName = "Substance", assayNumber = 1)
data_cleaned <- cleanData(D_list[[1]])

calculate_PLR(data_cleaned, calcContinuousPrelimRanges = FALSE)
```

calc_single_curve	<i>Calculate all necessary steps for a single calibration curve</i>
-------------------	---

Description

Calculate all necessary steps for a single calibration curve

Usage

```
calc_single_curve(
  D,
  substance = "substance",
  minReplicates = 3,
  cvThres = 20,
  calcContinuousPrelimRanges = FALSE,
  weightingMethod = "1/x^2",
  centralTendencyMeasure = "mean",
  perBiasThres = 20,
```

```

    considerPerBiasCV = TRUE,
    perBiasDistThres = 10,
    RfThresL = 80,
    RfThresU = 120
  )

```

Arguments

D	data.frame data set, e.g. result of readDataTable or readDataSE . Has to include exactly two columns: "Concentration" and "Measurement".
substance	character(1) Name of the substance (default is "substance"). Will be added to the result files and may be used when plotting multiple calibration curves in one plot.
minReplicates	integer(1) Minimal number of replicates per concentration level. Concentration levels with too few data points will be removed.
cvThres	numeric(1) Threshold for CV per concentration level in percent (default is 20).
calcContinuousPrelimRanges	logical(1) If TRUE, the longest continuous range is selected (default is TRUE). If FALSE, gaps with CVs larger than the threshold may be included.
weightingMethod	character(1) Method for weighting (currently "1/x", "1/x^2" and "None" are supported, default is 1/x^2).
centralTendencyMeasure	character(1) Method for calculating average percent bias, "mean" (default) or "median".
perBiasThres	numeric(1) Threshold for average percent bias in percent, default is 20.
considerPerBiasCV	logical(1) If TRUE, CV is considered for the elimination of the concentration level (default). CV will only be considered if the difference in percent bias values is lower than perBiasDistThres.
perBiasDistThres	numeric(1) Threshold for the difference in average percent bias in percent (for lower differences, CV will be considered), default is 10.
RfThresL	numeric(1) Lower threshold for response factor in percent (default is 80).
RfThresU	numeric(1) Upper threshold for response factor in percent (default is 120).

Value

List with the following elements:

- `mod`: lm-object containing the final linear model.
- `final_linear_range`: vector of concentration levels that are part of the final linear range.
- `weightingMethod`: weighting method used for the linear model.
- `result_table_conc_levels`: Result table with one line for each concentration level (generated by [assemble_results](#)).
- `result_table_obs`: Result table with one line per observation (e.g. individual response factors for each data point) (generated by [assemble_results](#)).

Examples

```
data_path <- system.file("extdata", "MSQC1.xlsx", "GGPFSDSYR_QTRAP_y5.xlsx",
  package = "CalibraCurve")
D <- readDataTable(dataPath = data_path, concCol = 16, measCol = 12,
  fileType = "xlsx")
calc_single_curve(D = D)
```

CalibraCurve

CalibraCurve

Description

CalibraCurve

Usage

```
CalibraCurve(
  D_list,
  output_path = NULL,
  substance = "substance",
  minReplicates = 3,
  cvThres = 20,
  calcContinuousPrelimRanges = FALSE,
  weightingMethod = "1/x^2",
  centralTendencyMeasure = "mean",
  perBiasThres = 20,
  considerPerBiasCV = TRUE,
  perBiasDistThres = 10,
  RfThresL = 80,
  RfThresU = 120,
  plot_type = "single_plots",
  RF_colour_threshold = "orange",
  RF_colour_within = "#00BFC4",
  RF_colour_outside = "#F8766D",
```

```

device = "png",
CC_plot_width = 15,
CC_plot_height = 10,
RF_plot_width = 15,
RF_plot_height = 10,
base_size = 11,
RF_legend = FALSE,
plot_dpi = 300,
verbose = TRUE,
...
)

```

Arguments

D_list	data.frame/list Data.frame or list of data.frames (one for one specific substance, each must contain two columns: Concentration and Measurement)
output_path	character(1) Folder to save results (table and plots). If NULL (default), results are not saved.
substance	character(1) Name of the substance (default is "substance1"). Will be added to the result files and will be used as labels in the plots.
minReplicates	integer(1) Minimal number of replicates/data points per concentration level. Concentration levels with too few data points will be removed.
cvThres	numeric(1) Threshold for CV per concentration level in percent (default is 20).
calcContinuousPrelimRanges	logical(1) If TRUE, the longest continuous range is selected (default is TRUE). If FALSE, gaps with CVs larger than the threshold may be included.
weightingMethod	character(1) Method for weighting (currently "1/x", "1/x^2" and "None" are supported, default is 1/x^2).
centralTendencyMeasure	character(1) Method for calculating average percent bias, "mean" (default) or "median".
perBiasThres	numeric(1) Threshold for average percent bias in percent, default is 20.
considerPerBiasCV	logical(1) If TRUE, CV is considered for the elimination of the concentration level (default). CV will only be considered if the difference in percent bias values is lower than perBiasDistThres.

perBiasDistThres	numeric(1) Threshold for the difference in average percent bias in percent (for lower differences, CV will be considered), default is 10.
RfThresL	numeric(1) Lower threshold for response factor in percent (default is 80).
RfThresU	numeric(1) Upper threshold for response factor in percent (default is 120).
plot_type	character(1) Type of plot for calibration curves: "single_plots" (default, generate a separate plot for each substance), "multiplot" (generate a graphic with subplots for each substance) or "all_in_one" (generate a single plot with all substances).
RF_colour_threshold	character(1) Response factor plot: Colour for horizontal threshold lines, default is "orange".
RF_colour_within	character(1) Response factor plot: Colour for points and lines within the final linear range, default is "#00BFC4" (default ggplot colour).
RF_colour_outside	character(1) Response factor plot: Colour for horizontal outside of the final linear range, default is "#F8766D" (default ggplot colour).
device	character(1) Device for saving the plot (default is "png"). Other options include "pdf", "jpeg", "tiff", "svg" etc. For details see ggsave .
CC_plot_width	numeric(1) Plot width in cm (default is 10).
CC_plot_height	numeric(1) Plot height in cm (default is 10).
RF_plot_width	numeric(1) Plot width in cm (default is 10).
RF_plot_height	numeric(1) Plot height in cm (default is 10).
base_size	numeric(1) Base size for the plot theme, default is 11.
RF_legend	logical(1) If TRUE, a legend will be added to the response factor plots.
plot_dpi	numeric(1) Plot resolution in dpi (default is 300).
verbose	logical(1) If FALSE, no messages will be printed.
...	additional parameters for plotCalibraCurve

Value

List with the following elements:

- RES: List of CalibraCurve results (one item per substance, output from `calc_single_curve`).
- summary_tab: Data.frame with summary information about the calibration curves, one row per substance.
- plot_CC_list: List of ggplot2 objects of the calibration curves (one per substance for "single_plots", otherwise only one item).
- plot_RF_list: List of ggplot2 objects of the response factor plots (one item).

Examples

```
### NOTE: as output_path is not specified here, no files will be saved.
### Set output_path to a folder of your choice to save the results.

### single xlsx file:
data_path <- system.file("extdata", "MSQC1_xlsx", "GGPFSDSYR_QTRAP_y5.xlsx",
  package = "CalibraCurve")
D <- readDataTable(dataPath = data_path, concCol = 16, measCol = 12,
  fileType = "xlsx")
RES <- CalibraCurve(D_list = D)
RES$plot_CC_list
RES$plot_RF_list

### multiple xlsx files (in a folder) as multiplot:
data_folder <- system.file("extdata", "MSQC1_xlsx", package = "CalibraCurve")
D_list <- readMultipleTables(dataFolder = data_folder, fileType = "xlsx",
  concCol = 16, measCol = 12)
RES <- CalibraCurve(D_list = D_list, plot_type = "multiplot")
RES$plot_CC_list

### single rds file (SummarizedExperiment) as an all-in-one plot:
file <- system.file("extdata", "MSQC1", "msqc1_dil_GGPFSDSYR.rds",
  package = "CalibraCurve")
D_list <- readDataSE(dataPath = file, concColName = "amount_fmol",
  substColName = "Substance", assayNumber = 1)
RES <- CalibraCurve(D_list, plot_type = "all_in_one")
RES$plot_CC_list
```

cleanData

Clean data (remove 0s and NAs, remove concentration levels with insufficient number of replicates)

Description

Clean data (remove 0s and NAs, remove concentration levels with insufficient number of replicates)

Usage

```
cleanData(rawData, minReplicates = 3)
```

Arguments

rawData	data.frame data set to be cleaned, result of readDataTable or readDataSE .
minReplicates	integer(1) Minimal number of replicates per concentration level. Concentration levels with too few data points will be removed.

Value

list of data.frames, each element contains data for a specific concentration level

Examples

```
file <- system.file("extdata", "MSQC1", "msqc1_dil_GGPFSDSYR.rds",
  package = "CalibraCurve"
)
D_list <- readDataSE(file,
  concColName = "amount_fmol",
  substColName = "Substance", assayNumber = 1
)
cleanData(D_list[[1]])
```

plotCalibraCurve

Plot the calibration curve

Description

Plot the calibration curve

Usage

```
plotCalibraCurve(
  CC_RES,
  ylab = "Intensity",
  xlab = "Concentration",
  show_regression_info = FALSE,
  show_linear_range = TRUE,
  show_data_points = TRUE,
  plot_type = "multiplot",
  point_colour = "black",
  curve_colour = "red",
  linear_range_colour = "black",
  multiplot_nrow = NULL,
```

```

    multiplot_ncol = NULL,
    multiplot_scales = "free",
    regression_info_size = 3,
    base_size = 11
  )

```

Arguments

CC_RES	list Results of CalibraCurve . Each list element is the result of calc_single_curve
ylab	character(1) y-axis label.
xlab	character(1) x-axis label.
show_regression_info	logical(1) If TRUE, show regression information (R2, slope, intercept) on the plot.
show_linear_range	logical(1) If TRUE, show the linear range of the calibration curve as a rectangle in the plot.
show_data_points	logical(1) If TRUE, show the data points on the plot.
plot_type	character(1) Type of plot for calibration curves: "single_plots" (default, generate a separate plot for each substance), "multiplot" (generate a graphic with subplots for each substance) or "all_in_one" (generate a single plot with all substances).
point_colour	character(1) Colour of the data points, default is "black".
curve_colour	character(1) Colour of the calibration curve, default is "red".
linear_range_colour	character(1) Colour of the linear range background, default is "black" (colour is weakened by $\alpha = 0.1$).
multiplot_nrow	integer(1) Number of rows for the multiplot layout (default is NULL, which means that there is only one row).
multiplot_ncol	integer(1) Number of columns for the multiplot layout (default is NULL, which means that the number of columns is determined automatically based on the number of curves).
multiplot_scales	character(1) Scales for the multiplot layout, default is "free" (which means that each plot has its own scales). Other options are "fixed", "free_x", "free_y".

regression_info_size	numeric(1) Size of the regression information text on the plot, default is 3.
base_size	numeric(1) Base size for the plot theme, default is 11.

Value

List of a ggplot2 object containing the calibration curve plot (CC_plot) and a data.frame containing summary data for annotations (annotation_dat).

Examples

```
file <- system.file("extdata", "MSQC1", "msqc1_dil_GGPFSDSYR.rds",
  package = "CalibraCurve"
)
D_list <- readDataSE(file,
  concColName = "amount_fmol",
  substColName = "Substance", assayNumber = 1
)
CC_RES <- calc_single_curve(D_list[[1]], calcContinuousPrelimRanges = FALSE)

plotCalibraCurve(list(substance = CC_RES))
```

plotResponseFactors	<i>Plot response factors</i>
---------------------	------------------------------

Description

Plot response factors

Usage

```
plotResponseFactors(
  RES,
  RfThresL = 80,
  RfThresU = 120,
  ylab = "Response Factor",
  xlab = "Concentration",
  colour_threshold = "orange",
  colour_within = "#00BFC4",
  colour_outside = "#F8766D",
  legend = FALSE,
  base_size = 11,
  substance = NULL
)
```

Arguments

RES	list Results of <code>calc_single_curve</code> .
RfThresL	numeric(1) Lower threshold for response factor in percent (default is 80).
RfThresU	numeric(1) Upper threshold for response factor in percent (default is 120).
ylab	character(1) y-axis label.
xlab	character(1) x-axis label.
colour_threshold	character(1) Colour for horizontal threshold lines, default is "orange".
colour_within	character(1) Colour for points and lines within the threshold, default is "#00BFC4" (default ggplot colour).
colour_outside	character(1) Colour for horizontal outside of the threshold, default is "#F8766D" (default ggplot colour).
legend	logical(1) If TRUE, a legend is added to the plot, default is FALSE.
base_size	numeric(1) Base size for the plot theme, default is 11.
substance	character(1) Name of the substance (default is "substance1"). Will be added to the result files and will be used as labels in the plots.

Value

A ggplot2 object containing the response factor plot.

Examples

```

file <- system.file("extdata", "MSQC1", "msqc1_dil_GGPFSDSYR.rds",
  package = "CalibraCurve"
)
D_list <- readDataSE(file,
  concColName = "amount_fmol",
  substColName = "Substance", assayNumber = 1
)
CC_RES <- calc_single_curve(D_list[[1]], calcContinuousPrelimRanges = FALSE)

plotResponseFactors(RES = CC_RES)

```

predictConcentration	<i>Predict concentrations from intensity values based on a given calibration curve</i>
----------------------	--

Description

Predict concentrations from intensity values based on a given calibration curve

Usage

```
predictConcentration(CC_res, newdata, verbose = TRUE)
```

Arguments

CC_res	list Results of CalibraCurve .
newdata	numeric A vector of intensity values for which to predict concentrations.
verbose	logical(1) If TRUE, a warning message is given if estimated concentrations are outside of the linear range.

Details

The function will give a warning if any of the predicted concentrations are outside the final linear range. This is important to ensure that the predictions are reliable and within the linear range of the calibration curve.

Value

A data frame with the following columns:

- **intensity**: The input intensity values.
- **predicted_concentrations**: The predicted concentrations based on the calibration curve.
- **linear_range**: A logical vector indicating whether the predicted concentrations are within the final linear range.

Examples

```
file <- system.file("extdata", "MSQC1", "msqc1_dil_GGPFSDSYR.rds",  
  package = "CalibraCurve")  
D <- readDataSE(file, concColName = "amount_fm1",  
  substColName = "Substance")  
RES <- CalibraCurve(D)  
newdata <- c(1000000, 10000000, 100000000) # 1e6, 1e7, 1e8  
predictConcentration(RE$RES[[4]], newdata = newdata)
```

readDataSE	<i>Read data stored as an SummarizedExperiment object (directly or stored in an .rds file). Extracts the two relevant columns (concentration and measurement) and orders the data by increasing concentration level.</i>
------------	--

Description

Read data stored as an SummarizedExperiment object (directly or stored in an .rds file). Extracts the two relevant columns (concentration and measurement) and orders the data by increasing concentration level.

Usage

```
readDataSE(  
  dataPath = NULL,  
  rawDataSE = NULL,  
  concColName,  
  substColName,  
  assayNumber = 1,  
  rowNumbers = NULL  
)
```

Arguments

dataPath	character(1) Path to the data file (.rds file)
rawDataSE	SummarizedExperiment SummarizedExperiment object
concColName	character(1) Name of the column in the colData() containing the concentration levels.
substColName	character(1) column name of rowData() containing the substance name (must be a unique value in each row)
assayNumber	integer(1) Number of assay to be extracted from the SummarizedExperiment object
rowNumbers	integer Row numbers to extract from the SummarizedExperiment object. Default is NULL, which means that all rows in the object will be used.

Details

The SummarizedExperiments object may contain quantitative values from targeted proteomics, lipidomics or metabolomics experiments. The colData has to contain a column with the concentration levels (concColName). The rowData has to contain a column with the substance names (e.g. peptide sequence, name of lipid or metabolite etc).

Value

List of data.frame, each with two numeric columns: Concentration and Measurement

Examples

```
file <- system.file("extdata", "MSQC1", "msqc1_dil_GGPFSDSYR.rds",
  package = "CalibraCurve")

D_list <- readDataSE(file,
  concColName = "amount_fmol",
  substColName = "Substance", assayNumber = 1)

# Alternative: import SummarizedExperiment object directly
rawDataSE <- readRDS(file)

D_list2 <- readDataSE(rawDataSE = rawDataSE,
  concColName = "amount_fmol",
  substColName = "Substance", assayNumber = 1
)
```

readDataTable	<i>Read data in different table input formats (xlsx, csv or txt). Extracts the two relevant columns (concentration and measurement) and orders the data by increasing concentration.</i>
---------------	--

Description

Read data in different table input formats (xlsx, csv or txt). Extracts the two relevant columns (concentration and measurement) and orders the data by increasing concentration.

Usage

```
readDataTable(
  dataPath,
  fileType,
  concCol,
  measCol,
  substCol = NULL,
  sep = ",",
  dec = ".",
  header = TRUE,
  naStrings = c("NA", "NaN", "Filtered", "#NV"),
  sheet = 1
)
```

Arguments

dataPath	character(1) Path to the data file (.csv, .txt or .xlsx file).
fileType	character(1) Type of file: "csv", "txt" or "xlsx".
concCol	integer(1) Column number of the concentration values.
measCol	integer Column number of the concentration values.
substCol	integer Column number of the substance names (optional). If not set, all rows will be interpreted as belonging to the same substance.
sep	character(1) The field separator, default is ",".
dec	character(1) Decimal separator, default is ".".
header	logical(1) If TRUE, first line is counted as column names. The default is TRUE.
naStrings	character Vector of strings which are to be interpreted as NA. The default is c("NA", "NaN", "Filtered", "#NV").
sheet	integer(1) Sheet number (only needed for xlsx files, default is to use the first sheet).

Value

Data.frame with two numeric columns: Concentration and Measurement

Examples

```
### xlsx file:
file <- system.file("extdata", "MSQC1_xlsx", "GGPFSDSYR_QTRAP_y5.xlsx",
  package = "CalibraCurve"
)
D <- readDataTable(file, fileType = "xlsx", concCol = 16, measCol = 12)
```

readMultipleTables	<i>Read folder of files in different table input formats (xlsx, csv or txt).</i>
--------------------	--

Description

Read folder of files in different table input formats (xlsx, csv or txt).

Usage

```
readMultipleTables(dataFolder, fileType, concCol, measCol, ...)
```

Arguments

dataFolder	character(1) Folder containing either xlsx, csv or txt files
fileType	character(1) Type of file: "csv", "txt" or "xlsx".
concCol	integer(1) Column number of the concentration values.
measCol	integer Column number of the concentration values.
...	additional parameters to readDataTable

Value

List of data.frame, each with two numeric columns: Concentration and Measurement

Examples

```
data_folder <- system.file("extdata", "MSQC1_xlsx",  
  package = "CalibraCurve")  
D_list <- readMultipleTables(  
  dataFolder = data_folder, fileType = "xlsx",  
  concCol = 16, measCol = 12  
)
```

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