Package 'CCWeights'

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Type Package

Title Perform Weighted Linear Regression for Calibration Curve

Version 0.1.6

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Description Automated assessment and selection of weighting factors for accurate quantification using linear calibration curve.
In addition, a 'shiny' App is provided, allowing users to analyze their data using an interactive graphical user interface, without any programming requirements.

Depends R (>= 3.5.0)

Imports plotly, dplyr, stats, magrittr, shiny, bs4Dash, fresh, DT, tools, readxl, rmarkdown, readr

License GPL-3

Encoding UTF-8

LazyData true

RoxygenNote 7.1.2

NeedsCompilation no

Repository CRAN

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R topics documented:

doCalibration *Perform Calibration*

Description

Perform calibration

Usage

```
doCalibration(DF, weights = NULL)
```

Arguments

DF	data frame, it must contain a column named 'Concentration' and a column named 'Response'
weights	default is NULL

Value

dataframe, the quantification result

Author(s)

Yonghui Dong

Examples

```
Concentration <- rep(c(10, 50, 100, "unknown"), each = 3)
Response <- c(133, 156, 177, 6650, 7800, 8850, 13300, 15600, 17700, 156, 1450, 1400)
DF <- cbind.data.frame(Concentration = Concentration, Response = Response)
result <- doCalibration(DF)
```

doEvaluation *Evaluate Different Weighting Factors*

Description

Evaluate different weighting factors.

Usage

```
doEvaluation(DF, p = 0.05, userWeights = NULL)
```

Arguments

DF	data frame, it must contain a column named 'Concentration' and a column named 'Response'
p	p-value, default is 0.05
userWeights	user defined weights in linear regression, default is NULL. User can easily define weights, e.g., "1/x", "1/x^2", "1/y"

Value

dataframe, weighting factor evaluation result

Author(s)

Yonghui Dong

Examples

```
Concentration <- rep(c(10, 50, 100, 500), each = 3)
Response <- c(133, 156, 177, 1300, 1450, 1600, 4000, 3881, 3700, 140000, 139000, 140000)
DF <- cbind.data.frame(Concentration = Concentration, Response = Response)
result <- doEvaluation(DF)
```

---

doFtest *Perform F Test*

Description

perform F test to evaluate homoscedasticity.

Usage

```
doFtest(DF, p = 0.01, lower.tail = FALSE)
```

Arguments

DF	data frame, it must contain a column named 'Concentration' and a column named 'Response'
p	p-value
lower.tail	default is FALSE

Value

dataframe, F test result

Author(s)

Yonghui Dong

Examples

```
Concentration <- rep(c(10, 50, 100, 500), each = 3)
Response <- c(133, 156, 177, 1300, 1450, 1600, 4000, 3881, 3700, 140000, 139000, 140000)
DF <- cbind.data.frame(Concentration, Response)
result <- doFtest(DF, p = 0.01)
```

---

doWlm *Perform Weighted Linear Regression*

Description

Perform weighted linear regression and evaluate by using summed residual.

Usage

```
doWlm(DF, weights = NULL)
```

Arguments

DF	data frame, it must contain a column named 'Concentration' and a column named 'Response'
weights	the weights used in linear regression, default is NULL. User can easily define weights, e.g., "1/x", "1/x^2", "1/y"

Value

list, weighted linear regression result

Author(s)

Yonghui Dong

Examples

```
Concentration <- rep(c(10, 50, 100, 500), each = 3)
Response <- c(133, 156, 177, 1300, 1450, 1600, 4000, 3881, 3700, 140000, 139000, 140000)
DF <- cbind.data.frame(Concentration = Concentration, Response = Response)
result <- doWlm(DF, weights = "1/x^2")
```

expData *expData*

Description

Two example data set: one with internal standards (IS), and one without IS

Usage

```
expData
```

Format

A list with 2 data frames:

noSTD the example data without IS

STD the example data with IS

runGui *Run CCWeights Gui*

Description

Run CCWeights Gui.

Usage

```
runGui()
```

Value

Gui

Author(s)

Yonghui Dong

Examples

```
if(interactive()){}
```

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