Package ‘MetaboQC’

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Type Package
Title Normalize Metabolomic Data using QC Signal
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Description Takes QC signal for each day and normalize metabolomic data that has been acquired in a certain period of time. At least three QC per day are required.
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graphQC  

*Represent the compounds area (normalized or not) as a function of their injection order to study trends.*

**Description**

Export graphs for each compound included in LCdata matrix in which the area of the specified compound is represented vs the injection order.

**Usage**

```r
graphQC(lcdata, g, NameDataSet)
```

**Arguments**

- **LCdata**: Matrix of data obtained (mainly by LC-MS) that included four data columns ("Compound Name","Order","QC","Day") and then one column for each compound or entity detected (normalized or not).
- **g**: Number of compounds for which the graph should be obtained.
- **NameDataSet**: A name for the data set that is going to be used for the pdf file name. It must be given in quotes.

**Value**

Multiple graphs of the compounds area (normalized or not) vs the injection order.

**Examples**

```r
## Not run:
graphQC(LCdata,3,"datasetName")
## End(Not run)
```

**QCCorrectionLOESS**  

*Generate values for metabolites normalization*

**Description**

According to the area of QC along each day, this function generates values for each sample injected along the day that are going to be used for data normalization.

**Usage**

```r
QCCorrectionLOESS(LCdata)
```
**QCcorrectionMultiLOESS**

**Arguments**

- **LCdata**: Matrix of data obtained (mainly by LC-MS) that included four data columns ("Compound Name","Order","QC","Day") and then one column for each compound or entity detected.

**Value**

A data set similar to LCdata matrix but with duplicated columns for each compound or entity with the area needed to normalize each of them.

**Examples**

```r
## Not run:
correctedLCdata <- QCcorrectionLOESS(LCdata)

## End(Not run)
```

---

**QCcorrectionMultiLOESS**

*Generate values for metabolites normalization*

**Description**

According to the area of QC along each day, this function generates values for each sample injected along the day that are going to be used for data normalization.

**Usage**

```r
QCcorrectionMultiLOESS(LCdata)
```

**Arguments**

- **LCdata**: Matrix of data obtained (mainly by LC-MS) that included four data columns ("Compound Name","Order","QC","Day") and then one column for each compound or entity detected.

**Value**

A data set similar to LCdata matrix but with duplicated columns for each compound or entity with the area needed to normalize each of them.

**Examples**

```r
## Not run:
correctedLCdata <- QCcorrectionMultiLOESS(LCdata)

## End(Not run)
```
QCcorrectionMultiPoly3

*Generate values for metabolites normalization*

**Description**

According to the area of QC along each day, this function generates values for each sample injected along the day that are going to be used for data normalization.

**Usage**

```
QCcorrectionMultiPoly3(LCdata)
```

**Arguments**

- **LCdata**
  
  Matrix of data obtained (mainly by LC-MS) that included four data columns ("Compound Name","Order","QC","Day") and then one column for each compound or entity detected.

**Value**

A data set similar to LCdata matrix but with duplicated columns for each compound or entity with the area needed to normalize each of them.

**Examples**

```R
# Not run:
correctedLCdata<-QCcorrectionMultiPoly3(LCdata)

# End(Not run)
```

---

QCcorrectionMultiPoly4

*Generate values for metabolites normalization*

**Description**

According to the area of QC along each day, this function generates values for each sample injected along the day that are going to be used for data normalization.

**Usage**

```
QCcorrectionMultiPoly4(LCdata)
```
Arguments

**LCdata**

Matrix of data obtained (mainly by LC-MS) that included four data columns ("Compound Name", "Order", "QC", "Day") and then one column for each compound or entity detected.

Value

A data set similar to LCdata matrix but with duplicated columns for each compound or entity with the area needed to normalize each of them.

Examples

```r
## Not run:
correctedLCdata <- QCcorrectionMultiPoly6(LCdata)

## End(Not run)
```

**Description**

According to the area of QC along each day, this function generates values for each sample injected along the day that are going to be used for data normalization.

**Usage**

```r
QCcorrectionMultiPoly6(LCdata)
```

Arguments

**LCdata**

Matrix of data obtained (mainly by LC-MS) that included four data columns ("Compound Name", "Order", "QC", "Day") and then one column for each compound or entity detected.

Value

A data set similar to LCdata matrix but with duplicated columns for each compound or entity with the area needed to normalize each of them.

Examples

```r
## Not run:
correctedLCdata <- QCcorrectionMultiPoly6(LCdata)

## End(Not run)
```
Description
According to the area of QC along each day, this function generates values for each sample injected along the day that are going to be used for data normalization.

Usage
QCcorrectionSinglePoly3(LCdata)

Arguments
- **LCdata**
  - Matrix of data obtained (mainly by LC-MS) that included four data columns ("Compound Name","Order","QC","Day") and then one column for each compound or entity detected.

Value
A data set similar to LCdata matrix but with duplicated columns for each compound or entity with the area needed to normalize each of them.

Examples
```r
## Not run:
correctedLCdata<-QCcorrectionSinglePoly3(LCdata)

## End(Not run)
```

---

Description
According to the area of QC along each day, this function generates values for each sample injected along the day that are going to be used for data normalization.

Usage
QCcorrectionSinglePoly4(LCdata)
Arguments
LCdata Matrix of data obtained (mainly by LC-MS) that included four data columns ("Compound Name","Order","QC","Day") and then one column for each compound or entity detected.

Value
A data set similar to LCdata matrix but with duplicated columns for each compound or entity with the area needed to normalize each of them.

Examples
## Not run:
correctedLCdata<-QCcorrectionSinglePoly6(LCdata)
## End(Not run)
QCregression

Equation to be used internally to predict values from a regression curve of grade 3

Description
Equation to be used internally to predict values from a regression curve of grade 3

Usage
QCregression(b, c, d, e, x)

Arguments
b coefficient from order 0 part of the equation
c coefficient from order 1 part of the equation
d coefficient from order 2 part of the equation
e coefficient from order 3 part of the equation
x the x-axis value from which the y-axis value wanted to be predicted for the equation given by the coefficients

Value
A y-value calculated for the x-value specified, taking into account the curve described by the coefficients given

Examples
```r
## Not run:
predictions <- QCregression(b, c, d, e, x)
## End(Not run)
#' @export
```

QCregression4

Equation to be used internally to predict values from a regression curve of grade 4

Description
Equation to be used internally to predict values from a regression curve of grade 4

Usage
QCregression4(b, c, d, e, f, x)
Arguments

- **b**: coefficient from order 0 part of the equation
- **c**: coefficient from order 1 part of the equation
- **d**: coefficient from order 2 part of the equation
- **e**: coefficient from order 3 part of the equation
- **f**: coefficient from order 4 part of the equation
- **x**: the x-axis value from which the y-axis value wanted to be predicted for the equation given by the coefficients

Value

A y-value calculated for the x-value specified, taking into account the curve described by the coefficients given

Examples

```r
## Not run:
prediction <- QCregression6(b, c, d, e, f, x)
## End(Not run)
```

Description

Equation to be used internally to predict values from a regression curve of grade 6

Usage

```r
QCregression6(b, c, d, e, f, g, h, x)
```

Arguments

- **b**: coefficient from order 0 part of the equation
- **c**: coefficient from order 1 part of the equation
- **d**: coefficient from order 2 part of the equation
- **e**: coefficient from order 3 part of the equation
- **f**: coefficient from order 4 part of the equation
- **g**: coefficient from order 5 part of the equation
- **h**: coefficient from order 6 part of the equation
- **x**: the x-axis value from which the y-axis value wanted to be predicted for the equation given by the coefficients
Value

A y-value calculated for the x-value specified, taking into account the curve described by the coefficients given.

Examples

```r
## Not run:
predictions <- QCregression6(b, c, d, e, f, g, h, x)

## End(Not run)
```
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