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.

License GPL-2

Depends R (>= 3.1.3)

Imports plyr

RoxygenNote 5.0.1

NeedsCompilation no

Repository CRAN

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Contents

`graphQC` *Representate 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

```
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 coulm 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

```
## 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

```
QCcorrectionLOESS(LCdata)
```

Arguments

`LCdata`	Matrix of data obtained (mainly by LC-MS) that included four data columns ("Compound Name","Order","QC","Day") and then one coulm 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<-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

```
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 coulm 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<-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 coulm 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<-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 coulm 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<-QCcorrectionMultiPoly4(LCdata)

## End(Not run)
```

`QCcorrectionMultiPoly6` *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

```
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 coulm 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<-QCcorrectionMultiPoly6(LCdata)

## End(Not run)
```

`QCcorrectionSinglePoly3` *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

```
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 coulm 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<-QCcorrectionSinglePoly3(LCdata)

## End(Not run)
```

`QCcorrectionSinglePoly4` *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

```
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 coulm 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<-QCcorrectionSinglePoly4(LCdata)

## End(Not run)
```

`QCcorrectionSinglePoly6`

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

```
QCcorrectionSinglePoly6(LCdata)
```

Arguments

`LCdata`	Matrix of data obtained (mainly by LC-MS) that included four data columns ("Compound Name","Order","QC","Day") and then one coulm 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 especified, taking into account the curve described by the coefficients given

Examples

```
## Not run:
prediction<-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 especified, taking into account the curve described by the coefficients given

Examples

```
## Not run:
prediction<-QCregression4(b,c,d,e,f,x)

## End(Not run)
```

`QCregression6` *Equation to be used internally to predict values from a regression curve of grade 6*

Description

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

Usage

```
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 especified, taking into account the curve described by the coefficients given

Examples

```
## Not run:
prediction<-QCregression4(b,c,d,e,f,g,h,x)

## End(Not run)
```

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