

Package: MetaboQC (via r-universe)

September 18, 2024

Type Package

Title Normalize Metabolomic Data using QC Signal

Version 1.1

Date 2021-09-22

Author Monica Calderon-Santiago

Maintainer Monica Calderon-Santiago <b42casam@uco.es>

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

Date/Publication 2021-09-29 11:00:06 UTC

Repository <https://monicacalsan.r-universe.dev>

RemoteUrl <https://github.com/cran/MetaboQC>

RemoteRef HEAD

RemoteSha ea51eeb3b73341179a44341fb837f777fb61c8e9

Contents

graphQC	2
QCcorrectionLOESS	3
QCcorrectionMultiLOESS	3
QCcorrectionMultiPoly3	4
QCcorrectionMultiPoly4	5
QCcorrectionMultiPoly6	5
QCcorrectionSinglePoly3	6
QCcorrectionSinglePoly4	7

QCcorrectionSinglePoly6	7
QCregression	8
QCregression4	9
QCregression6	10
Index	11

graphQC	<i>Representate the compounds area (normalized or not) as a function of their injection order to study trends.</i>
---------	--

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 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<-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 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<-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

```
## 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

```
## 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 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<-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 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<-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 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<-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 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	<i>Equation to be used internally to predict values from a regression curve of grade 3</i>
--------------	--

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

```
## Not run:  
prediction<-QCRegression(b,c,d,e,x)  
  
## End(Not run)  
#' @export
```

QCRegression4	<i>Equation to be used internally to predict values from a regression curve of grade 4</i>
---------------	--

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

```
## Not run:  
prediction<-QCRegression4(b,c,d,e,f,x)  
  
## End(Not run)
```

QCRegression6	<i>Equation to be used internally to predict values from a regression curve of grade 6</i>
---------------	--

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 specified, 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)
```

Index

graphQC, [2](#)

QCcorrectionLOESS, [3](#)

QCcorrectionMultiLOESS, [3](#)

QCcorrectionMultiPoly3, [4](#)

QCcorrectionMultiPoly4, [5](#)

QCcorrectionMultiPoly6, [5](#)

QCcorrectionSinglePoly3, [6](#)

QCcorrectionSinglePoly4, [7](#)

QCcorrectionSinglePoly6, [7](#)

QCregression, [8](#)

QCregression4, [9](#)

QCregression6, [10](#)