

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

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QCcorrectionLOESS	<i>Generate values for metabolites normalization</i>
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**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.
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### 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>
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**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>
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**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)
```

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