

# Package ‘pmp’

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**Type** Package

**Title** Peak Matrix Processing and signal batch correction for metabolomics datasets

**Version** 1.23.1

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**Description** Methods and tools for (pre-)processing of metabolomics datasets (i.e. peak matrices), including filtering, normalisation, missing value imputation, scaling, and signal drift and batch effect correction methods. Filtering methods are based on: the fraction of missing values (across samples or features); Relative Standard Deviation (RSD) calculated from the Quality Control (QC) samples; the blank samples. Normalisation methods include Probabilistic Quotient Normalisation (PQN) and normalisation to total signal intensity. A unified user interface for several commonly used missing value imputation algorithms is also provided. Supported methods are: k-nearest neighbours (knn), random forests (rf), Bayesian PCA missing value estimator (bpca), mean or median value of the given feature and a constant small value. The generalised logarithm (glog) transformation algorithm is available to stabilise the variance across low and high intensity mass spectral features. Finally, this package provides an implementation of the Quality Control-Robust Spline Correction (QCRSC) algorithm for signal drift and batch effect correction of mass spectrometry-based datasets.

**License** GPL-3

**biocViews** MassSpectrometry, Metabolomics, Software, QualityControl, BatchEffect

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|                       |                                         |
|-----------------------|-----------------------------------------|
| filter_peaks_by_blank | <i>Filter features by blank samples</i> |
|-----------------------|-----------------------------------------|

---

Description

Metabolomics datasets often contain many features of non-biological origin e.g. those associated with extraction and analysis solvents. This tool facilitates the removal of such features from the data matrix, as defined using an appropriate blank sample.

**Usage**

```
filter_peaks_by_blank(
  df,
  fold_change,
  classes,
  blank_label,
  qc_label = NULL,
  remove_samples = TRUE,
  remove_peaks = TRUE,
  fraction_in_blank = 0
)
```

**Arguments**

|                   |                                                                                                                                                                                                                                                             |
|-------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| df                | A matrix-like (e.g. an ordinary matrix, a data frame) or <a href="#">RangedSummarizedExperiment-class</a> object with all values of class <code>numeric()</code> or <code>integer()</code> of peak intensities, areas or other quantitative characteristic. |
| fold_change       | <code>numeric(1)</code> , fold_change minimum fold change between analytical and blank samples.                                                                                                                                                             |
| classes           | <code>character()</code> , vector of class labels. Must be the same length as the number of sample in the input peak table. If input is <code>SummarizedExperiment</code> object, use <code>SummarizedExperiment_object\$meta_data_column_name</code> .     |
| blank_label       | <code>character(1)</code> , class label used to identify blank samples.                                                                                                                                                                                     |
| qc_label          | <code>character(1)</code> or <code>NULL</code> , class label used to identify QC samples.                                                                                                                                                                   |
| remove_samples    | <code>logical(1)</code> , remove blank samples from peak matrix or not.                                                                                                                                                                                     |
| remove_peaks      | <code>logical(1)</code> , remove filtered features from peak matrix or not.                                                                                                                                                                                 |
| fraction_in_blank | <code>numeric(1)</code> , value between 0 to 1 to specify fraction in how many blanks peaks should be present.                                                                                                                                              |

**Details**

If parameter `qc_label` is not `NULL`, QC samples which will be used to calculate the median signal intensity.

**Value**

Object of class `SummarizedExperiment`. If input data are a matrix-like (e.g. an ordinary matrix, a data frame) object, function returns `numeric()` matrix-like object of filtered data set. Function flags are added to the object attributes and is a [DataFrame-class](#) with five columns. The same `DataFrame` object containing flags is added to `rowData()` element of `SummarizedExperiment` object as well.

Columns in `rowData()` or `flags` element contain:

median\_non\_blanks median intensities of features of non-blank samples;  
 median\_blanks median intensities of features of blank samples;  
 fold\_change fold change between analytical and blank samples;

blank\_flags integer(), if 0 feature is flagged to be removed;  
 blank\_fraction\_flags numeric(), fraction in how many blank samples peaks is present.

## Examples

```
df <- MTBLS79[,MTBLS79$Batch == 1]
df$Class[1:2] <- "Blank"
out <- filter_peaks_by_blank(df=df, fold_change=1.2,
  classes=df$Class, blank_label="Blank", qc_label=NULL,
  remove_samples=FALSE, remove_peaks=TRUE, fraction_in_blank=0)
```

---

filter\_peaks\_by\_fraction

*Filter features by fraction of missing values*

---

## Description

Metabolomics datasets often contain 'features' with irreproducible peak intensity values, or with large numbers of missing values. This tool facilitates the remove of such features from a data matrix, based upon the relative proportion (minimum fraction) of samples containing non-missing values.

## Usage

```
filter_peaks_by_fraction(
  df,
  min_frac,
  classes = NULL,
  method = "QC",
  qc_label = "QC",
  remove_peaks = TRUE
)
```

## Arguments

|              |                                                                                                                                                                                                                                   |
|--------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| df           | A matrix-like (e.g. an ordinary matrix, a data frame) or <a href="#">RangedSummarizedExperiment-class</a> object with all values of class numeric() or integer() of peak intensities, areas or other quantitative characteristic. |
| min_frac     | numeric(1), value between 0 and 1, a threshold of fraction of detection.                                                                                                                                                          |
| classes      | character(), vector of class labels. Must be the same length as the number of sample in the input peak table. If input is SummarizedExperiment object, use SummarizedExperiment_object\$meta_data_column_name.                    |
| method       | character(1), method to use. QC - within QC samples, within - within each sample class or across - across all samples.                                                                                                            |
| qc_label     | character(1) or NULL, class label used to identify QC samples.                                                                                                                                                                    |
| remove_peaks | logical(1), remove filtered features from peak matrix or not.                                                                                                                                                                     |

**Value**

Object of class SummarizedExperiment. If input data are a matrix-like (e.g. an ordinary matrix, a data frame) object, function returns `numeric()` matrix-like object of filtered data set. Function flags are added to the object attributes and is a [DataFrame-class](#) with five columns. The same DataFrame object containing flags is added to `rowData()` element of SummarizedExperiment object as well.

Columns in `rowData()` or `flags` element contain fractions of missing values per feature within QC samples (method QC), across (method across) or within (method within) each sample group.

**Examples**

```
df <- MTBLS79[,MTBLS79$Batch == 1]
out <- filter_peaks_by_fraction(df=df, min_frac=1,
  classes=df$class, method='QC', qc_label='QC')

out <- filter_peaks_by_fraction(df=df, min_frac=1,
  classes=df$class, method='across', qc_label='QC')

out <- filter_peaks_by_fraction(df=df, min_frac=1,
  classes=df$class, method='within', qc_label='QC')
```

---

|                     |                                              |
|---------------------|----------------------------------------------|
| filter_peaks_by_rsd | <i>Filter features by RSD% of QC samples</i> |
|---------------------|----------------------------------------------|

---

**Description**

Metabolomics datasets often contain 'features' with irreproducible peak intensity values, or with large numbers of missing values. This tool facilitates the remove of such features from a data matrix, based upon relative standard deviation of intensity values for a given feature within specified QC samples.

**Usage**

```
filter_peaks_by_rsd(df, max_rsd, classes, qc_label, remove_peaks = TRUE)
```

**Arguments**

|         |                                                                                                                                                                                                                                                             |
|---------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| df      | A matrix-like (e.g. an ordinary matrix, a data frame) or <a href="#">RangedSummarizedExperiment-class</a> object with all values of class <code>numeric()</code> or <code>integer()</code> of peak intensities, areas or other quantitative characteristic. |
| max_rsd | <code>numeric()</code> , threshold of QC RSD% value                                                                                                                                                                                                         |
| classes | <code>character()</code> , vector of class labels. Must be the same length as the number of sample in the input peak table. If input is SummarizedExperiment object, use <code>SummarizedExperiment_object\$meta_data_column_name</code> .                  |

|              |                                                                |
|--------------|----------------------------------------------------------------|
| qc_label     | character(1) or NULL, class label used to identify QC samples. |
| remove_peaks | logical(1), remove filtered features from peak matrix or not.  |

### Value

Object of class SummarizedExperiment. If input data are a matrix-like (e.g. an ordinary matrix, a data frame) object, function returns numeric() matrix-like object of filtered data set. Function flags are added to the object attributes and is a [DataFrame-class](#) with five columns. The same DataFrame-class object containing flags is added to rowData() element of SummarizedExperiment object as well.

Columns in rowData() or flags element contain:  
 rsd\_QC numeric(), RSD% value of QC samples per feature;  
 rsd\_flags integer(), if 0 feature is flagged to be removed.

### Examples

```
df <- MTBLS79[, MTBLS79$Batch == 1]
out <- filter_peaks_by_rsd(df=df, max_rsd=20,
  classes=df$class, qc_label='QC')
```

---

|                      |                                         |
|----------------------|-----------------------------------------|
| filter_samples_by_mv | <i>Filter samples by missing values</i> |
|----------------------|-----------------------------------------|

---

### Description

Missing values in mass spectrometry metabolomic datasets occur widely and can originate from a number of sources, including for both technical and biological reasons. In order for robust conclusions to be drawn from down-stream statistical testing procedures, the issue of missing values must first be addressed. This tool facilitates the removal of samples containing a user-defined maximum percentage of missing values.

### Usage

```
filter_samples_by_mv(df, max_perc_mv, classes = NULL, remove_samples = TRUE)
```

### Arguments

|                |                                                                                                                                                                                                                                   |
|----------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| df             | A matrix-like (e.g. an ordinary matrix, a data frame) or <a href="#">RangedSummarizedExperiment-class</a> object with all values of class numeric() or integer() of peak intensities, areas or other quantitative characteristic. |
| max_perc_mv    | numeric(1), Value between 0 and 1 of threshold of missing value percentage in sample.                                                                                                                                             |
| classes        | character(), vector of class labels. Must be the same length as the number of sample in the input peak table. If input is SummarizedExperiment object, use SummarizedExperiment_object\$meta_data_column_name.                    |
| remove_samples | logical(1), remove blank samples from peak matrix or not.                                                                                                                                                                         |

**Value**

Object of class SummarizedExperiment. If input data are a matrix-like (e.g. an ordinary matrix, a data frame) object, function returns numeric() matrix-like object of filtered data set. Function flags are added to the object attributes and is a [DataFrame-class](#) with five columns. The same DataFrame object containing flags is added to rowData() element of SummarizedExperiment object as well. If element colData() already exists flags are appended to existing values.

Columns in colData() or flags element contain:  
 perc\_mv numeric(), fraction of missing values per sample;  
 flags integer(), if 0 feature is flagged to be removed.

**Examples**

```
df <- MTBLS79
out <- filter_samples_by_mv (df=df, max_perc_mv=0.8)
```

---

glog\_plot\_optimised\_lambda

*Plot SSE error of lambda optimisation process*

---

**Description**

Plot SSE error of lambda optimisation process

**Usage**

```
glog_plot_optimised_lambda(
  df,
  optimised_lambda,
  classes,
  qc_label,
  plot_grid = 100
)
```

**Arguments**

|                  |                                                                                                                                                                                                                                   |
|------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| df               | A matrix-like (e.g. an ordinary matrix, a data frame) or <a href="#">RangedSummarizedExperiment-class</a> object with all values of class numeric() or integer() of peak intensities, areas or other quantitative characteristic. |
| optimised_lambda | numeric(1), value of optimised lambda from glog_transformation output.                                                                                                                                                            |
| classes          | character(), vector of class labels. Must be the same length as the number of sample in the input peak table. If input is SummarizedExperiment object, use SummarizedExperiment_object\$meta_data_column_name.                    |

qc\_label            character(1) or NULL, class label used to identify QC samples.  
 plot\_grid          integer(1), number of data points to use for SSE optimisation.

### Value

Class ggplot object containing optimisation plot.

### Examples

```
data <- MTBLS79[, MTBLS79$Batch == 1]
classes <- data$Class

data <- mv_imputation(df=data, method='knn')
out <- glog_transformation (df=data, classes=classes,
  qc_label='QC')

optimised_lambda <- S4Vectors::metadata(out)
optimised_lambda <-
  optimised_lambda$processing_history$glog_transformation$lambda_opt

glog_plot_optimised_lambda(df=data, classes=classes,
  qc_label="QC", optimised_lambda=optimised_lambda)
```

---

|                     |                                                                         |
|---------------------|-------------------------------------------------------------------------|
| glog_transformation | <i>Variance stabilising generalised logarithm (glog) transformation</i> |
|---------------------|-------------------------------------------------------------------------|

---

### Description

Performs glog transformation on the data set. QC samples can be used to estimate technical variation in the data set and calculate transformation parameter  $\lambda$  (lambda). QC samples usually comprise a pool of aliquots taken from all other samples in the study and analysed repeatedly throughout an analytical batch.

### Usage

```
glog_transformation(df, classes, qc_label, lambda = NULL)
```

### Arguments

|          |                                                                                                                                                                                                                                                             |
|----------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| df       | A matrix-like (e.g. an ordinary matrix, a data frame) or <a href="#">RangedSummarizedExperiment-class</a> object with all values of class <code>numeric()</code> or <code>integer()</code> of peak intensities, areas or other quantitative characteristic. |
| classes  | <code>character()</code> , vector of class labels. Must be the same length as the number of sample in the input peak table. If input is <code>SummarizedExperiment</code> object, use <code>SummarizedExperiment_object\$meta_data_column_name</code> .     |
| qc_label | <code>character(1)</code> or <code>NULL</code> , class label used to identify QC samples.                                                                                                                                                                   |
| lambda   | <code>NULL</code> or <code>numeric(1)</code> , if not <code>NULL</code> will use provided value for glog lambda.                                                                                                                                            |

## Details

Many univariate and multivariate statistical tests require homogeneity and normality of dataset variance. Real-world metabolomics datasets often fail to meet these criteria due to asymmetric (i.e. non-'normal') and/or heteroscedatic (i.e. non-homogenous) variance structure. To address this issue, glog data transformations may be applied.

For each cell within the data matrix, transform the raw value (x) according to:  $\log_{10}(x + \sqrt{x^2 + \lambda})$ . The parameter  $\lambda$  is typically calculated using quality control (QC) samples analysed throughout an analysis batch.

## Value

Object of class SummarizedExperiment. If input data are a matrix-like (e.g. an ordinary matrix, a data frame) object, function returns the same R data structure as input with all value of data type numeric().

## References

Parsons HM et. al., BMC Bioinf., 8(234), 2007. <https://doi.org/10.1186/1471-2105-8-234>

## Examples

```
df <- MTBLS79[, MTBLS79$Batch == 1]
out <- mv_imputation(df=df, method="knn")
out <- glog_transformation (df=out, classes=df$Class,
  qc_label="QC")
```

---

MTBLS79

*Direct-infusion mass spectrometry (DIMS) data set*


---

## Description

Data set of 20 biological (cow vs sheep) serum samples that were analysed repeatedly, in 8 batches across 7 days.

## Usage

MTBLS79

## Format

A [RangedSummarizedExperiment-class](#) object.

assay(MTBLS79) Peak intensities of the DIMS data set. Contains 172 samples and 2488 features.

colData(MTBLS79) Sample meta data containing 4 columns.

Batch - character(), sample batch name.

Sample\_Rep - character(), sample replicate code.

Class - character(), sample class labels.

Class2 - character(), alternative sample class labels grouping together replicate samples.

## Details

Code below includes all commands used to generate MTBLS79 object.

```
library (openxlsx)
library (SummarizedExperiment)

download.file(destfile = "MTBLS79.xlsx", mode="wb",
url = "ftp://ftp.ebi.ac.uk/pub/databases/metabolights/studies/public/
  MTBLS79/Dataset07__SFPM.xlsx")
wb <- openxlsx::loadWorkbook(xlsxFile="MTBLS79.xlsx")

MTBLS79 <- list()

MTBLS79$assay <- openxlsx::readWorkbook(wb, "data", colNames=T, rowNames=T)

# Last row of the peak matrix represent mean intensities across all samples.
MTBLS79$assay <- MTBLS79$assay[-c(nrow(MTBLS79$assay)), ]

# Transpose peak matrix, so that features are in rows and samples in columns.
MTBLS79$assay <- as.matrix(t(MTBLS79$assay))

# Missing values in the input data are stored as 0, replace with NA
MTBLS79$assay[MTBLS79$assay == 0] <- NA

rownames(MTBLS79$assay) <- round(as.numeric(rownames(MTBLS79$assay)), 5)

MTBLS79$colData <- openxlsx::readWorkbook(wb, "meta", colNames=T, rowNames=F)
MTBLS79$colData <- MTBLS79$colData[-c(nrow(MTBLS79$colData)), 1:4]

MTBLS79 <- SummarizedExperiment(assays=list(MTBLS79$assay),
colData=DataFrame(MTBLS79$colData))
```

## Source

<https://www.ebi.ac.uk/metabolights/MTBLS79>

## References

Kirwan et al, Scientific Data volume 1, Article number: 140012 (2014) <https://www.nature.com/articles/sdata201412>

## Description

Missing values in metabolomics data sets occur widely and can originate from a number of sources, including technical and biological reasons.

Missing values imputation is applied to replace non-existing values with an estimated values while maintaining the data structure. A number of different methods are available as part of this function.

## Usage

```
mv_imputation(  
  df,  
  method,  
  k = 10,  
  rowmax = 0.5,  
  colmax = 0.5,  
  maxp = NULL,  
  check_df = TRUE  
)
```

## Arguments

|          |                                                                                                                                                                                                                                                             |
|----------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| df       | A matrix-like (e.g. an ordinary matrix, a data frame) or <a href="#">RangedSummarizedExperiment-class</a> object with all values of class <code>numeric()</code> or <code>integer()</code> of peak intensities, areas or other quantitative characteristic. |
| method   | <code>character(1)</code> , missing value imputation method. Supported methods are <code>knn</code> , <code>rf</code> , <code>bpca</code> , <code>sv</code> , <code>'mn'</code> and <code>'md'</code> .                                                     |
| k        | <code>numeric(1)</code> , for a given sample containing a missing value, the number of nearest neighbours to include to calculate a replacement value. Used only for method <code>knn</code> .                                                              |
| rowmax   | <code>numeric(1)</code> , the maximum percentage of missing data allowed in any row. For any rows exceeding given limit, missing values are imputed using the overall mean per sample. Used only for method <code>knn</code> .                              |
| colmax   | <code>numeric(1)</code> , the maximum percent missing data allowed in any column. If any column exceeds given limit, the function will report an error Used only for method <code>knn</code> .                                                              |
| maxp     | <code>integer(1)</code> , number of features to run on single core. If set to <code>NULL</code> will use total number of features.                                                                                                                          |
| check_df | <code>logical(1)</code> , if set to <code>TRUE</code> will check if input data needs to be transposed, so that features are in rows.                                                                                                                        |

## Details

Supported missing value imputation methods are:

`knn` - K-nearest neighbour. For each feature in each sample, missing values are replaced by the mean average value (non-weighted) calculated from its k closest neighbours in multivariate space (default distance metric: euclidean distance);

rf - Random Forest. This method is a wrapper of [missForest](#) function. For each feature, missing values are iteratively imputed until a maximum number of iterations (10), or until the difference between consecutively-imputed matrices becomes positive. Trees per forest are set to 100, variables included per tree are calculate using formula  $\sqrt{totalnumberofvariables}$ ;

bPCA - Bayesian principal component analysis. This method is a wrapper of [pca](#) function. Missing values are replaced by the values obtained from principal component analysis regression with a Bayesian method. Therefore every imputed missing value does not occur multiple times, neither across the samples nor across the metabolite features;

sv - Small value. For each feature, replace missing values with half of the lowest value recorded in the entire data matrix;

'mn' - Mean. For each feature, replace missing values with the mean average (non-weighted) of all other non-missing values for that variable;

'md' - Median. For each feature, replace missing values with the median of all other non-missing values for that variable.

## Value

Object of class SummarizedExperiment. If input data are a matrix-like (e.g. an ordinary matrix, a data frame) object, function returns the same R data structure as input with all value of data type numeric().

## Examples

```
df <- MTBLS79[,MTBLS79$Batch == 1]
out <- mv_imputation(df=df, method='knn')
```

---

normalise\_to\_sum

*Normalisation by total sum of the features per sample*

---

## Description

For each sample, every feature intensity value is divided by the total sum of all feature intensity values measured in that sample (NA values ignored by default), before multiplication by 100; the unit is %.

## Usage

```
normalise_to_sum(df, check_df = TRUE)
```

## Arguments

|          |                                                                                                                                                                                                                                                             |
|----------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| df       | A matrix-like (e.g. an ordinary matrix, a data frame) or <a href="#">RangedSummarizedExperiment-class</a> object with all values of class <code>numeric()</code> or <code>integer()</code> of peak intensities, areas or other quantitative characteristic. |
| check_df | <code>logical(1)</code> , if set to <code>TRUE</code> will check if input data needs to be transposed, so that features are in rows.                                                                                                                        |

## Value

Object of class `SummarizedExperiment`. If input data are a matrix-like (e.g. an ordinary matrix, a data frame) object, function returns the same R data structure as input with all value of data type `numeric()`.

## Examples

```
df <- MTBLS79[,MTBLS79$Batch == 1]
out <- normalise_to_sum (df=df)
```

---

|                   |                                                   |
|-------------------|---------------------------------------------------|
| pqn_normalisation | <i>Probabilistic quotient normalisation (PQN)</i> |
|-------------------|---------------------------------------------------|

---

## Description

For every feature the mean response is calculated across all QC samples. A reference vector is then generated. The median between the reference vector and every sample is computed obtaining a vector of coefficients related to each sample. Each sample is then divided by the median value of the vector of coefficients; this median value is different for each sample. This method was adapted by Dieterle et al. (2006) (see references). Its purpose is to take into account the concentration changes of some metabolite features that affect limited regions of the data.

## Usage

```
pqn_normalisation(
  df,
  classes,
  qc_label,
  ref_mean = NULL,
  qc_frac = 0,
  sample_frac = 0,
  ref_method = "mean"
)
```

**Arguments**

|             |                                                                                                                                                                                                                                                             |
|-------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| df          | A matrix-like (e.g. an ordinary matrix, a data frame) or <a href="#">RangedSummarizedExperiment-class</a> object with all values of class <code>numeric()</code> or <code>integer()</code> of peak intensities, areas or other quantitative characteristic. |
| classes     | <code>character()</code> , vector of class labels. Must be the same length as the number of sample in the input peak table. If input is <code>SummarizedExperiment</code> object, use <code>SummarizedExperiment_object\$meta_data_column_name</code> .     |
| qc_label    | <code>character(1)</code> or <code>NULL</code> , class label used to identify QC samples.                                                                                                                                                                   |
| ref_mean    | <code>numeric()</code> or <code>NULL</code> , Vector of reference mean values to use instead of calculating from QC sample group. If set to <code>NULL</code> , QC sample data will be used.                                                                |
| qc_frac     | <code>numeric()</code> A value between 0 and 1 to indicate the minimum proportion of QC samples a feature must be present in for it to be included when computing the reference. Default <code>qc_frac = 0</code> .                                         |
| sample_frac | <code>numeric()</code> A value between 0 and 1 to indicate the minimum proportion of samples a feature must be present in for it to be considered when computing the normalisation coefficients. Default <code>sample_frac = 0</code> .                     |
| ref_method  | <code>character()</code> Method used to compute the reference from the QC samples. Default <code>ref_method = 'mean'</code> . Allowed values are "mean" or "median".                                                                                        |

**Value**

Object of class `SummarizedExperiment`. If input data are matrix-like (e.g. an ordinary matrix, a data frame) object, the same R data structure as the input will be returned with all values of the data type.

`numeric()`.

**References**

Dieterle F. et al., Anal. Chem., 78(13), 2006. <http://dx.doi.org/10.1021/ac051632c>

**Examples**

```
df <- MTBLS79[ , MTBLS79$Batch==1]
pqn_normalisation(df=df,
  classes=df$Class, qc_label='QC')
```

---

processing\_history      *Return history of applied functions and argument from pmp package.*

---

**Description**

Return history of applied functions and argument from pmp package.

**Usage**

```
processing_history(df)
```

**Arguments**

**df** A matrix-like (e.g. an ordinary matrix, a data frame) or [RangedSummarizedExperiment-class](#) object with all values of class `numeric()` or `integer()` of peak intensities, areas or other quantitative characteristic.

**Value**

List of function names and argument values.

**Examples**

```
df <- MTBLS79[,MTBLS79$Batch == 1]
df$Class[1:2] <- "Blank"
out <- filter_peaks_by_blank(df=df, fold_change=1.2,
  classes=df$Class, blank_label="Blank", qc_label=NULL,
  remove_samples=FALSE, remove_peaks=TRUE, fraction_in_blank=0)
processing_history(out)
```

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QCRSC

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*Quality Control-Robust Spline Correction (QC-RSC)*


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**Description**

Implementation of Quality QC-RSC algorithm for signal drift and batch effect correction within/across a multi-batch direct infusion mass spectrometry (DIMS) and liquid chromatography mass spectrometry (LCMS) datasets. This version supports missing values, but requires at least 4 data point for quality control (QC) samples measured within each analytical batch. The smoothing parameter (`spar`) can be optimised using leave-one-out cross validation to avoid overfitting.

**Usage**

```
QCRSC(
  df,
  order,
  batch,
  classes,
  spar = 0,
  log = TRUE,
  minQC = 5,
  qc_label = "QC",
  spar_lim = c(-1.5, 1.5)
)
```

**Arguments**

|                       |                                                                                                                                                                                                                                                             |
|-----------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <code>df</code>       | A matrix-like (e.g. an ordinary matrix, a data frame) or <a href="#">RangedSummarizedExperiment-class</a> object with all values of class <code>numeric()</code> or <code>integer()</code> of peak intensities, areas or other quantitative characteristic. |
| <code>order</code>    | <code>numeric()</code> , A numeric vector indicating the order in which samples were measured.                                                                                                                                                              |
| <code>batch</code>    | <code>numeric()</code> or <code>character()</code> , a vector indicating the batch each sample was measured in. If only one batch was measured then all values should be set to 1                                                                           |
| <code>classes</code>  | <code>character()</code> , vector of class labels. Must be the same length as the number of sample in the input peak table. If input is <code>SummarizedExperiment</code> object, use <code>SummarizedExperiment_object\$meta_data_column_name</code> .     |
| <code>spar</code>     | <code>numeric(1)</code> , Spline smoothing parameter. Should be in the range 0 to 1. If set to 0 it will be estimated using leave-one-out cross-validation.                                                                                                 |
| <code>log</code>      | <code>logical(1)</code> , to perform the signal correction fit on the log scaled data. Default is TRUE.                                                                                                                                                     |
| <code>minQC</code>    | <code>integer(1)</code> , Minimum number of measured quality control (QC) samples required for signal correction within feature per batch. For features where signal was measured in less QC samples than threshold signal correction won't be applied.     |
| <code>qc_label</code> | <code>character(1)</code> or NULL, class label used to identify QC samples.                                                                                                                                                                                 |
| <code>spar_lim</code> | A 2 element numeric vector containing the min and max values of <code>spar</code> when searching for an optimum. Default <code>spar_lim = c(-1.5, 1.5)</code>                                                                                               |

**Value**

Object of class `SummarizedExperiment`. If input data are a matrix-like (e.g. an ordinary matrix, a data frame) object, function returns the same R data structure as input with all value of data type `numeric()`.

**Author(s)**

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**References**

Kirwan et al, Anal. Bioanal. Chem., 405 (15), 2013 <https://dx.doi.org/10.1007/s00216-013-6856-7>

**Examples**

```
classes <- MTBLS79$Class
batch <- MTBLS79$Batch
order <- c(1:ncol(MTBLS79))

out <- QCRSC(df = MTBLS79[1:10, ], order = order, batch = MTBLS79$Batch,
classes = MTBLS79$Class, spar = 0, minQC = 4)
```

---

|              |                                                   |
|--------------|---------------------------------------------------|
| remove_peaks | <i>Remove features from peak intensity matrix</i> |
|--------------|---------------------------------------------------|

---

**Description**

Filter to remove features.

**Usage**

```
remove_peaks(df, rem_index)
```

**Arguments**

|           |                                                                                                                                                                                                                                                             |
|-----------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| df        | A matrix-like (e.g. an ordinary matrix, a data frame) or <a href="#">RangedSummarizedExperiment-class</a> object with all values of class <code>numeric()</code> or <code>integer()</code> of peak intensities, areas or other quantitative characteristic. |
| rem_index | <code>logical()</code> , vector containing TRUE vales for features to remove. Should be the same length as number of features in input data.                                                                                                                |

**Value**

Object of class `SummarizedExperiment`. If input data are a matrix-like (e.g. an ordinary matrix, a data frame) object, function returns the same R data structure as input with all value of data type `numeric()`.

**Examples**

```
df <- MTBLS79[,MTBLS79$Batch == 1]
rem_index <- vector(mode="logical",
  length=nrow(SummarizedExperiment::assay(df)))
rem_index[c(1, 20, 456, 789)] <- TRUE
out <- remove_peaks(df=df, rem_index=rem_index)
```

---

|          |                                     |
|----------|-------------------------------------|
| sbc_plot | <i>Plot QCRSC corrected outputs</i> |
|----------|-------------------------------------|

---

**Description**

Plot the output from signal batch correction for the selected or the first 100 features.

**Usage**

```
sbc_plot(
  df,
  corrected_df,
  classes,
  batch,
  indexes = NULL,
  qc_label = "QC",
  output = "sbcms_plots.pdf"
)
```

**Arguments**

|              |                                                                                                                                                                                                                                                             |
|--------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| df           | A matrix-like (e.g. an ordinary matrix, a data frame) or <a href="#">RangedSummarizedExperiment-class</a> object with all values of class <code>numeric()</code> or <code>integer()</code> of peak intensities, areas or other quantitative characteristic. |
| corrected_df | Output from <a href="#">QCRSC</a> function.                                                                                                                                                                                                                 |
| classes      | <code>character()</code> , vector of class labels. Must be the same length as the number of sample in the input peak table. If input is <code>SummarizedExperiment</code> object, use <code>SummarizedExperiment_object\$meta_data_column_name</code> .     |
| batch        | <code>numeric()</code> or <code>character()</code> , a vector indicating the batch each sample was measured in. If only one batch was measured then all values should be set to 1                                                                           |
| indexes      | <code>numeric()</code> , a vector defining which features to plot. If set to <code>NULL</code> will plot the first 100.                                                                                                                                     |
| qc_label     | <code>character(1)</code> or <code>NULL</code> , class label used to identify QC samples.                                                                                                                                                                   |
| output       | <code>character()</code> , a filename of the output pdf file. Can include the path. If set to <code>NULL</code> output will be list object containing class <code>ggplot</code> plots.                                                                      |

**Value**

Pdf file or `list()` object `ggplot` class showing data before and after signal correction.

**Examples**

```
order <- c(1:ncol(MTBLS79))
data <- MTBLS79[1:10, ]

out <- QCRSC(df =data, order=order, batch=MTBLS79$Batch,
  classes=MTBLS79$Class, spar=0, minQC=4)
plots <- sbc_plot (df=data, corrected_df=out, classes=MTBLS79$Class,
  batch=MTBLS79$Batch, output=NULL)
```

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