

Package ‘MSstatsQC’

April 8, 2025

Version 2.25.0

Type Package

Title Longitudinal system suitability monitoring and quality control
for proteomic experiments

Description MSstatsQC is an R package which provides longitudinal system suitability monitoring and quality control tools for proteomic experiments.

License Artistic License 2.0

LazyData TRUE

URL <http://msstats.org/msstatsqc>

BugReports <https://groups.google.com/forum/#!forum/msstatsqc>

RoxygenNote 7.1.0

Imports dplyr,plotly,ggplot2,ggExtra, stats,grid, MSnbase, qcmetrics

Suggests knitr,rmarkdown, testthat, RforProteomics

VignetteBuilder knitr

biocViews Software, QualityControl, Proteomics, MassSpectrometry

git_url <https://git.bioconductor.org/packages/MSstatsQC>

git_branch devel

git_last_commit 0ea25be

git_last_commit_date 2024-10-29

Repository Bioconductor 3.21

Date/Publication 2025-04-07

Author Eralp Dogu [aut, cre],
Sara Taheri [aut],
Olga Vitek [aut]

Maintainer Eralp Dogu <eralp.dogu@gmail.com>

Contents

| | |
|--------------------------------|-----------|
| ChangePointEstimator | 2 |
| CUSUMChart | 3 |
| DataProcess | 5 |
| DecisionMap | 6 |
| MissingDataMap | 7 |
| MSnbaseToMSstatsQC | 8 |
| QCloudDDA | 8 |
| QCloudSRM | 9 |
| QuiCDIA | 10 |
| RadarPlot | 10 |
| RemoveMissing | 11 |
| RiverPlot | 12 |
| S9Site54 | 13 |
| XmRChart | 14 |
| Index | 16 |

| | |
|----------------------|---|
| ChangePointEstimator | <i>A function to identify the time of a change in the mean or variability of a metric</i> |
|----------------------|---|

Description

A function to identify the time of a change in the mean or variability of a metric

Usage

```
ChangePointEstimator(
  data = NULL,
  peptide,
  L = 1,
  U = 5,
  metric,
  normalization = TRUE,
  ytitle = "Change Point Plot - mean",
  type = "mean",
  selectMean = NULL,
  selectSD = NULL
)
```

Arguments

| | |
|---------|---|
| data | comma-separated (.csv), metric file. It should contain a "Precursor" column and the metrics columns. It should also include "Annotations" for each observation. |
| peptide | the name of precursor of interest. |
| L | Lower bound of the guide set. |

| | |
|---------------|--|
| U | Upper bound of the guide set. |
| metric | the name of metric of interest. |
| normalization | TRUE metric is standardized and FALSE if not standardized. |
| ytitle | the y-axis title of the plot. Defaults to "Change Point Plot - mean". The x-axis title is by default "QCno-name of peptide" |
| type | the type of the control chart. Two values can be assigned, "mean" or "variability". Default is "mean". |
| selectMean | the mean of a metric. It is used when mean is known. It is NULL when mean is not known. The default is NULL. |
| selectSD | the standard deviation of a metric. It is used when standard deviation is known. It is NULL when mean is not known. The default is NULL. |

Value

A plot of likelihood statistics versus time per peptide and metric generated from `CP.data.prepare` data frame.

Examples

```
# First process the data to make sure it's ready to use
sampleData <- DataProcess(S9Site54)
head(sampleData)
# Find the name of the peptides
levels(sampleData$Precursor)
# Calculate change point statistics
ChangePointEstimator(data = sampleData, peptide = "VLVLDTDYK", metric = "BestRetentionTime")
ChangePointEstimator(data = sampleData, peptide = "VLVLDTDYK", metric = "BestRetentionTime",
  ytitle = "Change Point Plot - variability", type = "variability")
ChangePointEstimator(data = sampleData, peptide = "VLVLDTDYK", metric = "BestRetentionTime",
  selectMean = 27.78, selectSD = 8.19)
ChangePointEstimator(data = sampleData, peptide = "DDGSWEVIEGYR", metric = "TotalArea")
ChangePointEstimator(data = sampleData, peptide = "DDGSWEVIEGYR", metric = "TotalArea",
  selectMean = 35097129, selectSD = 34132861)
ChangePointEstimator(data = sampleData, peptide = "TAAYVNAIEK", metric = "MaxFWHM")
```

| | |
|------------|---|
| CUSUMChart | <i>A function to create cumulative sum charts for mean (CUSUMm) and cumulative sum charts for variability (CUSUMv) control charts</i> |
|------------|---|

Description

A function to create cumulative sum charts for mean (CUSUMm) and cumulative sum charts for variability (CUSUMv) control charts

Usage

```

CUSUMChart(
  data = NULL,
  peptide,
  L = 1,
  U = 5,
  metric,
  normalization = TRUE,
  ytitle = "CUSUMm",
  type = "mean",
  selectMean = NULL,
  selectSD = NULL,
  referenceValue = 0.5,
  decisionInterval = 5
)

```

Arguments

| | |
|-------------------------------|---|
| <code>data</code> | comma-separated (.csv), metric file. It should contain a "Precursor" column and the metrics columns. It should also include "Annotations" for each observation. |
| <code>peptide</code> | the name of precursor of interest. |
| <code>L</code> | Lower bound of the guide set. |
| <code>U</code> | Upper bound of the guide set. |
| <code>metric</code> | the name of metric of interest. |
| <code>normalization</code> | TRUE if metric is standardized and FALSE if not standardized. |
| <code>ytitle</code> | the y-axis title of the plot. Defaults to "CUSUMm". The x-axis title is by default "Time : name of peptide" |
| <code>type</code> | the type of the control chart. Two values can be assigned, "mean" or "variability". Default is "mean" |
| <code>selectMean</code> | the mean of a metric. It is used when mean is known. It is NULL when mean is not known. The default is NULL. |
| <code>selectSD</code> | the standard deviation of a metric. It is used when standard deviation is known. It is NULL when mean is not known. The default is NULL. |
| <code>referenceValue</code> | the value that is used to tune the control chart for a proper shift size |
| <code>decisionInterval</code> | the threshold to detect an out-of-control observation |

Value

A plot of positive and negative CUSUM statistics versus time per peptide and metric generated from CUSUM.data.prepare data frame.

Examples

```
# First process the data to make sure it's ready to use
sampleData <- DataProcess(S9Site54)
head(sampleData)
# Find the name of the peptides
levels(sampleData$Precursor)
# Calculate CUSUM statistics
CUSUMChart(data = sampleData, peptide = "VLVLDTDYK", metric = "BestRetentionTime")
CUSUMChart(data = sampleData, peptide = "VLVLDTDYK", metric = "BestRetentionTime",
  ytitle = "CUSUMv", type = "variability")
CUSUMChart(data = sampleData, peptide = "VLVLDTDYK", metric = "BestRetentionTime",
  selectMean = 27.78, selectSD = 8.19)
CUSUMChart(data = sampleData, peptide = "DDGSWEVIEGYR", metric = "TotalArea")
CUSUMChart(data = sampleData, peptide = "DDGSWEVIEGYR", metric = "TotalArea",
  selectMean = 35097129, selectSD = 34132861)
CUSUMChart(data = sampleData, peptide = "TAAYVNAIEK", metric = "MaxFWHM")
```

| | |
|-------------|-----------------------------------|
| DataProcess | <i>A data processing function</i> |
|-------------|-----------------------------------|

Description

A data processing function

Usage

```
DataProcess(data = NULL)
```

Arguments

data Comma-separated (*.csv), QC file format. It should contain a Precursor column and the metrics columns.

Value

A data frame that processes using `input.sanity.check` function.

Examples

```
# The data is "S9Site54" which is defined in the package.
data <- DataProcess(S9Site54)
```

| | |
|-------------|--|
| DecisionMap | <i>A function to create heatmaps to compare performance with user defined performance criteria</i> |
|-------------|--|

Description

A function to create heatmaps to compare performance with user defined performance criteria

Usage

```
DecisionMap(
  data = NULL,
  method = "XmR",
  peptideThresholdRed = 0.7,
  peptideThresholdYellow = 0.5,
  L = 1,
  U = 5,
  type = "mean",
  title = "heatmap plot",
  listMean = NULL,
  listSD = NULL
)
```

Arguments

| | |
|------------------------|--|
| data | Comma-separated (*.csv), QC file format. It should contain a Precursor column and the metrics columns. |
| method | It is either "CUSUM" or "XmR" |
| peptideThresholdRed | Is a threshold that marks percentage of peptides above it red on the heatmap. Defaults to 0.7 |
| peptideThresholdYellow | Is a threshold that marks percentage of peptides above it and below the peptide-ThresholdRed, yellow on the heatmap. Defaults to 0.5 |
| L | Lower bound of the guide set. Defaults to 1 |
| U | Upper bound of the guide set. Defaults to 5 |
| type | can take two values, "mean" or "dispersion". Defaults to "mean" |
| title | the title of the plot. Defaults to "heatmap plot" |
| listMean | List of the means for the metrics. If you don't know the means leave it as NULL and they will be calculated automatically by using L and U. The default is NULL. |
| listSD | List of the standard deviations for the metrics. If you don't know the standard deviations leave it as NULL and they will be calculated automatically by using L and U. The default is NULL. |

Value

A heatmap to aggregate results per metric generated from heatmap.DataFrame data frame.

Examples

```
# First process the data to make sure it's ready to use
sampleData <- DataProcess(S9Site54)
head(sampleData)
# Draw Decision maker plot
DecisionMap(data = sampleData, method = "CUSUM")
DecisionMap(data = sampleData, method = "CUSUM", type = "variability")
DecisionMap(data = sampleData, method = "XmR")
DecisionMap(data = sampleData, method = "XmR", type = "variability")
```

| | |
|----------------|---|
| MissingDataMap | <i>A function to summarize missing values</i> |
|----------------|---|

Description

A function to summarize missing values

Usage

```
MissingDataMap(data)
```

Arguments

| | |
|------|----------------|
| data | Processed data |
|------|----------------|

Value

A plot of missing values.

Examples

```
# The data is "S9Site54" which is defined in the package.
data <- DataProcess(S9Site54)
MissingDataMap(data)
```

MSnbaseToMSstatsQC *A function to convert MSnbase files to MSstatsQC format*

Description

A function to convert MSnbase files to MSstatsQC format

Usage

```
MSnbaseToMSstatsQC(msfile)
```

Arguments

msfile data file to be converted

Value

A data frame that can be used with MSstatsQC

A csv file that is converted from raw files

Examples

```
## Not run: library(RforProteomics)
## Not run: msfile <- getPXD000001mzXML()
## Not run: MSnbaseToMSstatsQC(msfile)
```

QCloudDDA *DDA QC data from QCloud System*

Description

QC results generated from QCloud system

Usage

```
data(QCloudDDA)
```

Format

csv

Details

DDA QC data from QCloud System

Value

An example dataset generated from QCloud system

Examples

```
head(QCloudDDA)
```

QCloudSRM

SRM QC data from QCloud System

Description

QC results generated from QCloud system

Usage

```
data(QCloudSRM)
```

Format

csv

Details

SRM QC data from QCloud System

Value

An example dataset generated from QCloud system

Examples

```
head(QCloudSRM)
```

`QuiCDIA`*DIA iRT data from QuiC System*

Description

QC results generated from QuiC system

Usage

```
data(QuiCDIA)
```

Format

csv

Details

DIA iRT data from QuiC System

Value

An example dataset generated from QuiC system

Examples

```
head(QuiCDIA)
```

`RadarPlot`*A function to create radar plot to aggregate results from X and mR charts or CUSUMm and CUSUMv charts.*

Description

A function to create radar plot to aggregate results from X and mR charts or CUSUMm and CUSUMv charts.

Usage

```
RadarPlot(  
  data = NULL,  
  L = 1,  
  U = 5,  
  method = "XmR",  
  listMean = NULL,  
  listSD = NULL  
)
```

Arguments

| | |
|----------|--|
| data | omma-separated (.csv), metric file. It should contain a "Precursor" column and the metrics columns. It should also include "Annotations" for each observation. |
| L | lower bound of the guide set. |
| U | upper bound of the guide set. |
| method | defines the method selected to construct control charts. |
| listMean | list of the means for each metric. It is used when mean is known. It is NULL when mean is not known. The default is NULL. |
| listSD | list of the standard deviations for each metric. It is used when standard deviation is known. It is NULL when mean is not known. The default is NULL. automatically by using L and U. The default is NULL. |

Value

A radar plot to aggregate results per metric generated from `XmR.Radar.Plot.DataFrame` data frame or `CUSUM.Radar.Plot.DataFrame` data frame.

Examples

```
# First process the data to make sure it's ready to use
sampleData <- DataProcess(S9Site54)
head(sampleData)
# Draw XmR radar plot
RadarPlot(data = sampleData)
RadarPlot(data = sampleData, method = "CUSUM")
RadarPlot(data = sampleData,
           listMean = list("BestRetentionTime" = 27.78,
                           "TotalArea" = 35097129,
                           "MaxFWHM" = 0.28,
                           "MinStartTime" = 24),
           listSD = list("BestRetentionTime" = 8.19,
                          "TotalArea" = 34132861,
                          "MaxFWHM" = 0.054,
                          "MinStartTime" = 24)
           )
```

RemoveMissing

A data processing function for removing missing values

Description

A data processing function for removing missing values

Usage

```
RemoveMissing(data = NULL)
```

Arguments

`data` Comma-separated (*.csv), QC file format. It should contain a Precursor column and the metrics columns.

Value

A data frame that processes using `input.sanity.check` function.

Examples

```
# The data is "S9Site54" which is defined in the package.
data <- RemoveMissing(S9Site54)
```

| | |
|-----------|---|
| RiverPlot | <i>A function to create river plot to aggregate results from X and mR charts or CUSUMm and CUSUMv charts.</i> |
|-----------|---|

Description

A function to create river plot to aggregate results from X and mR charts or CUSUMm and CUSUMv charts.

Usage

```
RiverPlot(
  data = NULL,
  L = 1,
  U = 5,
  method = "XmR",
  listMean = NULL,
  listSD = NULL
)
```

Arguments

`data` comma-separated (.csv), metric file. It should contain a "Precursor" column and the metrics columns. It should also include "Annotations" for each observation.

`L` lower bound of the guide set.

`U` upper bound of the guide set.

`method` defines the method selected to construct control charts.

`listMean` list of the means for each metric. It is used when mean is known. It is NULL when mean is not known. The default is NULL.

`listSD` list of the standard deviations for each metric. It is used when standard deviation is known. It is NULL when mean is not known. The default is NULL.

Value

A river plot to aggregate results per metric generated from XmR.Summary.DataFrame data frame or CUSUM.Summary.DataFrame data frame.

Examples

```
# First process the data to make sure it's ready to use
sampleData <- DataProcess(S9Site54)
head(sampleData)
# Draw XmR summary plot
RiverPlot(data = sampleData)
RiverPlot(data = sampleData, L=1, U=20, method = "XmR",
          listMean = list("BestRetentionTime" = 27.78,
                          "TotalArea" = 35097129,
                          "MaxFWHM" = 0.28,
                          "MinStartTime" = 24),
          listSD = list("BestRetentionTime" = 8.19,
                        "TotalArea" = 34132861,
                        "MaxFWHM" = 0.054,
                        "MinStartTime" = 24)
          )
```

S9Site54

CPTAC study 9.1 site 54 dataset

Description

system suitability testing results generated during CPTAC Study 9.1 for Site 54

Usage

```
data(S9Site54)
```

Format

csv

Details

CPTAC system suitability testing data for Site 54 from Study 9.1

Value

An example dataset generated from CPTAC study 9.1

References

<http://www.mcponline.org/content/early/2015/02/18/mcp.M114.047050>

Examples

```
head(S9Site54)
```

| | |
|----------|--|
| XmRChart | <i>A function to construct individual (X) and moving range (mR) control charts</i> |
|----------|--|

Description

A function to construct individual (X) and moving range (mR) control charts

Usage

```
XmRChart(
  data = NULL,
  peptide,
  L = 1,
  U = 5,
  metric,
  normalization = FALSE,
  ytitle = "Individual observations",
  type = "mean",
  selectMean = NULL,
  selectSD = NULL
)
```

Arguments

| | |
|---------------|---|
| data | comma-separated (.csv), metric file. It should contain a "Precursor" column and the metrics columns. It should also include "Annotations" for each observation. |
| peptide | the name of precursor of interest. |
| L | Lower bound of the guide set. |
| U | Upper bound of the guide set. |
| metric | the name of metric of interest. |
| normalization | TRUE if metric is standardized and FALSE if not standardized. |
| ytitle | the y-axis title of the plot. Defaults to "Individual observations". The x-axis title is by default "Time : name of peptide" |
| type | the type of the control chart. Two values can be assigned, "mean" or "variability". Default is "mean". |
| selectMean | the mean of a metric. It is used when mean is known. It is NULL when mean is not known. The default is NULL. |
| selectSD | the standard deviation of a metric. It is used when standard deviation is known. It is NULL when mean is not known. The default is NULL. |

Value

A plot of individual values or moving ranges versus time per peptide and metric generated from XmR.data.prepare data frame.

Examples

```
# First process the data to make sure it's ready to use
sampleData <- DataProcess(S9Site54)
head(sampleData)
# Find the name of the peptides
levels(sampleData$Precursor)
# Calculate X and mR statistics
XmRChart(data = sampleData, peptide = "VLVLDTDYK", metric = "BestRetentionTime")
XmRChart(data = sampleData, peptide = "VLVLDTDYK", metric = "BestRetentionTime",
          ytitle = "moving ranges", type = "variability")
XmRChart(data = sampleData, peptide = "VLVLDTDYK", metric = "BestRetentionTime",
          selectMean = 27.78, selectSD = 8.19)
XmRChart(data = sampleData, peptide = "DDGSWEVIEGYR", metric = "TotalArea")
XmRChart(data = sampleData, peptide = "DDGSWEVIEGYR", metric = "TotalArea",
          selectMean = 35097129, selectSD = 34132861)
XmRChart(data = sampleData, peptide = "TAAYVNAIEK", metric = "MaxFWHM")
XmRChart(data = sampleData, peptide = "LVNELTEFAK", metric = "MinStartTime")
```

Index

- * **MSnbase**,
 - MSnbaseToMSstatsQC, 8
 - * **Sum**,
 - CUSUMChart, 3
 - * **XmR**,
 - XmRChart, 14
 - * **XmR**
 - RadarPlot, 10
 - RiverPlot, 12
 - * **change**
 - ChangePointEstimator, 2
 - * **chart**
 - ChangePointEstimator, 2
 - CUSUMChart, 3
 - XmRChart, 14
 - * **control**
 - ChangePointEstimator, 2
 - CUSUMChart, 3
 - XmRChart, 14
 - * **cumulative**
 - CUSUMChart, 3
 - * **datasets**
 - QCloudDDA, 8
 - QCloudSRM, 9
 - QuiCDIA, 10
 - S9Site54, 13
 - * **heatmap**
 - DecisionMap, 6
 - * **input**
 - MSnbaseToMSstatsQC, 8
 - * **point**,
 - ChangePointEstimator, 2
 - * **qcmetrics**,
 - MSnbaseToMSstatsQC, 8
- ChangePointEstimator, 2
- CUSUMChart, 3
- DataProcess, 5
- DecisionMap, 6
- MissingDataMap, 7
- MSnbaseToMSstatsQC, 8
- QCloudDDA, 8
- QCloudSRM, 9
- QuiCDIA, 10
- RadarPlot, 10
- RemoveMissing, 11
- RiverPlot, 12
- S9Site54, 13
- XmRChart, 14