Package 'hdxmsqc'

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Type Package

Title An R package for quality Control for hydrogen deuterium exchange mass spectrometry experiments

Version 1.5.0

Description The hdxmsqc package enables us to analyse and visualise the quality of HDX-MS experiments. Either as a final quality check before downstream analysis and publication or as part of a interative procedure to determine the quality of the data. The package builds on the QFeatures and Spectra packages to integrate with other mass-spectrometry data.

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Encoding UTF-8

LazyData false

Depends R(>= 4.3), QFeatures, S4Vectors, Spectra

Imports dplyr, tidyr, ggplot2, BiocStyle, knitr, methods, grDevices, stats, MsCoreUtils

Suggests RColorBrewer, pheatmap, MASS, patchwork, testthat

VignetteBuilder knitr

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biocViews QualityControl,DataImport, Proteomics, MassSpectrometry, Metabolomics

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Contents

`BRD4df` *This is data to be included in my package*

Description

A small HDX-MS dataset for BRD4 in apo state and in complex with IBET151

Author(s)

My Name <ococrook@gmail.com>

`BRD4df_full` *This is data to be included in my package*

Description

A complete HDX-MS dataset for BRD4 in apo state and in complex with IBET151

Author(s)

My Name <ococrook@gmail.com>

chargeCorrelationHdx *Charge states should have correlated incorperation but they need not be exactly the same*

Description

Charge states should have correlated incorperation but they need not be exactly the same

Usage

```
chargeCorrelationHdx(object, experiment = NULL, timepoints = NULL)
```

Arguments

object	An object of class QFeatures
experiment	A character vector indicating the experimental conditions
timepoints	A numeric vector indicating the experimental timepoints

Author(s)

Oliver Crook

Examples

```
data("BRD4df_full")
BRD4df_filtered <- isMissingAtRandom(object = BRD4df_full)
BRD4df_full_imputed <- impute(BRD4df_filtered, method = "zero", i = 1)
experiment <- c("wt", "iBET")
timepoints <- rep(c(0, 15, 60, 600, 3600, 14000), each = 3)
monoStat <- chargeCorrelationHdx(object = BRD4df_full_imputed,
experiment = experiment,
timepoints = timepoints)
```

compatibleUptake *Check whether deuterium uptakes are compatible with difference overlapping sequences.*

Description

Check whether deuterium uptakes are compatible with difference overlapping sequences.

Usage

```
compatibleUptake(object, overlap = 5, experiment = NULL, timepoints = NULL)
```

Arguments

object	An object of class QFeatures
overlap	How much overlap is required to check consistentcy. Default is sequences within 5 residues
experiment	A character vector indicating the experimental conditions
timepoints	A numeric vector indicating the experimental timepoints

Author(s)

Oliver Crook

Examples

```
data("BRD4df")
result <- compatibleUptake(BRD4df,  experiment = 1, timepoints = 1)
```

---

computeMassError *Empirical versus theoretical mass errors*

Description

Empirical versus theoretical mass errors

Usage

```
computeMassError(object, eCentroid = "Exp.Cent", tCentroid = "Theor.Cent")
```

Arguments

object	An object of class QFeatures
eCentroid	character string indicating column identifier for experimental centroid
tCentroid	character string indicating column identifier for theoretical centroid

Value

The error difference between the empirical and theoretical centroid

Author(s)

Oliver Crook

Examples

```
data("BRD4df")
result <- computeMassError(BRD4df, "Exp.Cent", "Theor.Cent")
head(result)
```

computeMonotoneStats *Monotonicity based outlier detection.*

Description

Monotonicity based outlier detection.

Usage

```
computeMonotoneStats(object, experiment = NULL, timepoints = NULL)
```

Arguments

object	An object of class QFeatures
experiment	A character vector indicating the experimental conditions
timepoints	A numeric vector indicating the experimental timepoints

Author(s)

Oliver Crook

Examples

```
data("BRD4df")
result <- computeMonotoneStats(BRD4df, experiment = 1, timepoint = 1)
```

exchangeableAmides *Compute exchangeable amides.*

Description

Computes the number of exchangeable amides based on the sequnece

Usage

```
exchangeableAmides(sequence)
```

Arguments

sequence	The sequence of the peptide

Value

Returns a numeric indicating the number of exchangeable amides

Examples

```
exchangeableAmides(sequence = "HDAEHAHEAPRKL")
```

`fourierIsotope` *fourier transform approach to computing isotopic distribution*

Description

fourier transform approach to computing isotopic distribution

Usage

```
fourierIsotope(
  elements,
  incorp = 0,
  num_exch_sites = 0,
  charge = 1,
  isotopes = NULL
)
```

Arguments

`elements`	A list of elements
`incorp`	The deuterium incoperation
`num_exch_sites`	The number of exchangable amides. Default is 0.
`charge`	The charge state of the peptide
`isotopes`	The number of isotopes to compute. The default is NULL, in whiich a default heuristic is used to make a good guess that covers the expected peaks.

Value

A list of mass and intensity value corresponding to the isotope distribution

Author(s)

Oliver Crook

Examples

```
fourierIsotope(c(C = 0, H = 2, N = 0, O = 1, S = 0, P = 0))
```

`generateSpectra` *generate Spectra using a fourier transform*

Description

generate Spectra using a fourier transform

Usage

```
generateSpectra(
  sequences,
  incorps,
  charges,
  customs = list(code = NULL, elements = NULL)
)
```

Arguments

`sequences`	A vector of peptide sequences
`incorps`	A vector of deuterium incoperation
`charges`	A vector of charge states of the peptide
`customs`	Custom elements supplied as a list

Value

A Spectra object corresponding to the isotope distributions

Author(s)

Oliver Crook

Examples

```
generateSpectra(sequence = "HDAEHAHEAPRKL", incorps = c(0.5), charges = 2)
```

`hdxmsqc` *A package to perfrom quality control for mass-spectrometry based hydrogen deuterium exchange experiment.*

Description

'hdxmsqc' provides the functionality to assess the quality and perform quality control of HDX-MS experiments. Raw and processed data can be visualized and analyzed to identify potential issues with the data. The package is designed to work with data from any HDX-MS platform. Typically, users will have exported results from either HDExaminer or DynamX software. There is not need to filter the data in either of those software systems.

Author(s)

Oliver Crook

imTimeOutlier *Ion Mobility time based outlier analysis*

Description

Ion Mobility time based outlier analysis

Usage

```
imTimeOutlier(
  object,
  rightIMS = "rightIMS",
  leftIMS = "leftIMS",
  searchIMS = "Search.IMS"
)
```

Arguments

object	An object of class QFeatures
rightIMS	A string indicating the right boundary of the ion mobility separation time. Defaults is "rightIMS".
leftIMS	A string indicating the left boundary of the ion mobility separation time. Default is "leftIMS".
searchIMS	A string indicating the actual ion mobility search time. The default is "Search.IMS"

Author(s)

Oliver Crook

Examples

```
data("BRD4df_full")
BRD4df_filtered <- isMissingAtRandom(object = BRD4df_full)
BRD4df_full_imputed <- impute(BRD4df_filtered, method = "zero", i = 1)
imTimeOutlier(object = BRD4df_full_imputed)
```

intensityOutliers *Intensity based deviations*

Description

Intensity based deviations

Usage

```
intensityOutliers(object, fcolIntensity = "Max.Inty")
```

Arguments

object	An object of class QFeatures
fcolIntensity	character to intensity intensity columns. Default is "Max.Inty" and uses regular expressions to find relevant columns

Value

The Cook's distance to characterise outleirs

Author(s)

Oliver Crook

Examples

```
data("BRD4df_full")

intensityOutliers(BRD4df_full)
```

---

isMissingAtRandom *Missing at random versus missing not at random*

Description

Missing at random versus missing not at random

Usage

```
isMissingAtRandom(object, threshold = NULL, filter = TRUE)
```

Arguments

object	An object of class QFeatures
threshold	A threshold indicated how many missing values indicate whether missingness is not at random. Default is NULL, which means leads to a threshold which is half the number of columns.
filter	A logial indicating whether to filter out data that is deemed missing not at random data("BRD4df_full") isMissingAtRandom(BRD4df_full)

Value

Adds a missing not at random indicator column

Author(s)

Oliver Crook

isotopicDistributionHDXfourier *fourier transform approach to computing isotopic distribution*

Description

fourier transform approach to computing isotopic distribution

Usage

```
isotopicDistributionHDXfourier(
  sequence,
  incorp = 0,
  charge = 1,
  custom = list(code = NULL, elements = NULL)
)
```

Arguments

sequence	A peptide
incorp	The deuterium incoperation
charge	The charge state of the peptide
custom	custom amino acids can be provided here provide a list of the elements.

Value

A list of mass and intensity value corresponding to the isotope distribution

Author(s)

Oliver Crook

Examples

```
isotopicDistributionHDXfourier(sequence = "HDAEHAHEAPRKL")
```

plotImTimeOutlier *Ion Mobility time based outlier analysis*

Description

Ion Mobility time based outlier analysis

Usage

```
plotImTimeOutlier(
  object,
  rightIMS = "rightIMS",
  leftIMS = "leftIMS",
  searchIMS = "Search.IMS"
)
```

Arguments

object	An object of class QFeatures
rightIMS	A string indicating the right boundary of the ion mobility separation time. Defaults is "rightIMS".
leftIMS	A string indicating the left boundary of the ion mobility separation time. Default is "leftIMS".
searchIMS	A string indicating the actual ion mobility search time. The default is "Search.IMS"

Author(s)

Oliver Crook

Examples

```
library(RColorBrewer)
data("BRD4df_full")
BRD4df_filtered <- isMissingAtRandom(object = BRD4df_full)
BRD4df_full_imputed <- impute(BRD4df_filtered, method = "zero", i = 1)
plotImTimeOutlier(object = BRD4df_full_imputed)
```

---

plotIntensityOutliers *Intensity based deviation plot*

Description

Intensity based deviation plot

Usage

```
plotIntensityOutliers(object, fcolIntensity = "Max.Inty")
```

Arguments

object	An object of class QFeatures
fcolIntensity	character to intensity intensity columns. Default is "Max.Inty" and uses regular expressions to find relevant columns

Value

A ggplot2 object showing intensity based outliers

Author(s)

Oliver Crook

Examples

```
data("BRD4df_full")
library(RColorBrewer)

plotIntensityOutliers(BRD4df_full)
```

plotMassError *Mass error plot*

Description

Mass error plot

Usage

```
plotMassError(object, eCentroid = "Exp.Cent", tCentroid = "Theor.Cent")
```

Arguments

object	An object of class QFeatures
eCentroid	character string indicating column identifier for experimental centroid
tCentroid	character string indicating column identifier for theoretical centroid

Value

a ggplot2 object which can be used to visualise the

Author(s)

Oliver Crook

Examples

```
library(RColorBrewer)
data("BRD4df")
result <- plotMassError(BRD4df, "Exp.Cent", "Theor.Cent")
```

plotMissing *missing value plot*

Description

missing value plot

Usage

```
plotMissing(object, ...)
```

Arguments

object	An object of class QFeatures
...	Additional arguemnts to pheatmap

Value

a pheatmap showing missing values

Author(s)

Oliver Crook

Examples

```
data("BRD4df_full")
library(pheatmap)
library(RColorBrewer)

plotMissing(BRD4df_full)
```

`plotMonotoneStat` *Monotonicity based outlier detection, plot.*

Description

Monotonicity based outlier detection, plot.

Usage

```
plotMonotoneStat(object, experiment = NULL, timepoints = NULL)
```

Arguments

`object`	An object of class `QFeatures`
`experiment`	A character vector indicating the experimental conditions
`timepoints`	A numeric vector indicating the experimental timepoints

Author(s)

Oliver Crook

Examples

```
library("RColorBrewer")
data("BRD4df_full")
experiment <- c("wt", "iBET")
timepoints <- rep(c(0, 15, 60, 600, 3600, 14000), each = 3)
monoStat <- computeMonotoneStats(object = BRD4df_full,
experiment = experiment,
timepoints = timepoints)
```

`plotrTimeOutliers` *Retention time based analysis*

Description

Retention time based analysis

Usage

```
plotrTimeOutliers(
  object,
  leftRT = "leftRT",
  rightRT = "rightRT",
  searchRT = "Search.RT"
)
```

Arguments

`object`	An object of class `QFeatures`
`leftRT`	A character indicated pattern associated with left boundary of retention time search. Default is "leftRT".
`rightRT`	A character indicated pattern associated with right boundary of retneton time search. Default is "rightRT".
`searchRT`	The actual search retention time pattern. Default is "Search.RT"

Value

a ggplot2 object showing distribution of retention time windows.

Author(s)

Oliver Crook

Examples

```
data("BRD4df_full")
library(RColorBrewer)

plotrTimeOutliers(BRD4df_full)
```

processHDE *Function to curate and HDExaminer file so that in contains all the information in a sensible format. This object can then be straightforwardly passed to a object of class* QFeatures

Description

Function to curate and HDExaminer file so that in contains all the information in a sensible format. This object can then be straightforwardly passed to a object of class QFeatures

Usage

```
processHDE(HDExaminerFile, proteinStates = NULL)
```

Arguments

HDExaminerFile	an object of class data.frame containing an HDExaminer data
proteinStates	a character vector indicating the protein states

Value

A wide format data frame with HDExaminer data

Author(s)

Oliver Crook

Examples

```
sample_data <- data.frame(read.csv(system.file("extdata", "ELN55049_AllResultsTables_Uncurated.csv", package

processHDE(sample_data)
```

qualityControl *Quality Control table function. Generate a table that collates quality control metrics*

Description

Quality Control table function. Generate a table that collates quality control metrics

Usage

```
qualityControl(
  object,
  massError = NULL,
  intensityOutlier = NULL,
  retentionOutlier = NULL,
  monotonicityStat = NULL,
  mobilityOutlier = NULL,
  chargeCorrelation = NULL,
  replicateCorrelation = NULL,
  replicateOutlier = NULL,
  sequenceCheck = NULL,
  spectraCheck = NULL,
  experiment = NULL,
  timepoints = NULL,
  undeuterated = FALSE
)
```

Arguments

object	An object of class Qfeatures, with the data used for the analysis
massError	The output of the computeMassError function
intensityOutlier	The output of the intensityOutliers function
retentionOutlier	The output of the rTimeOutliers function
monotonicityStat	The output of the computeMonotoneStats function
mobilityOutlier	The output of the imTimeOutliers function
chargeCorrelation	The output of the chargeCorrelationsHdx function
replicateCorrelation	The output of the replicateCorrelation function
replicateOutlier	The output of the replicateOutlier function
sequenceCheck	The output of the compatibleUptake function
spectraCheck	The output of the spectraSimiarity function
experiment	The experimental conditions.
timepoints	The timepoints used in the analysis, must include repeat for replicates
undeuterated	A logical indicating whether only the undeuterated data should be exported

Value

An object of class DataFrame containing a summary of the quality control results.

Author(s)

Oliver Crook

`replicateCorrelation` *Correlation based checks*

Description

Correlation based checks

Usage

```
replicateCorrelation(object, experiment, timepoints)
```

Arguments

`object`	An object of class QFeatures.
`experiment`	A character vector indicating the experimental conditions
`timepoints`	A numeric vector indicating the experimental timepoints

Value

Returns A list of the same length as the number of experiments indicating outlier from correlation analysis. Outliers are flagged if their deuterium uptake is highly variable.

Author(s)

Oliver Crook

Examples

```
data("BRD4df_full")
experiment <- c("wt", "iBET")
timepoints <- rep(c(0, 15, 60, 600, 3600, 14000), each = 3)
monoStat <- replicateCorrelation(object = BRD4df_full,
experiment = experiment,
timepoints = timepoints)
```

`replicateOutlier` *Correlation based checks*

Description

Correlation based checks

Usage

```
replicateOutlier(object, experiment, timepoints)
```

Arguments

object	An object of class QFeatures.
experiment	A character vector indicating the experimental conditions
timepoints	A numeric vector indicating the experimental timepoints

Value

Returns A list of the same length as the number of experiments indicating outlier from correlation analysis. Outliers are flagged if their deuterium uptake is highly variable.

Author(s)

Oliver Crook

Examples

```
data("BRD4df_full")
BRD4df_filtered <- isMissingAtRandom(object = BRD4df_full)
BRD4df_full_imputed <- impute(BRD4df_filtered, method = "zero", i = 1)
experiment <- c("wt", "iBET")
timepoints <- rep(c(0, 15, 60, 600, 3600, 14000), each = 3)
monoStat <- replicateOutlier(object = BRD4df_full_imputed,
experiment = experiment,
timepoints = timepoints)
```

---

rTimeOutliers *Retention time based analysis*

Description

Retention time based analysis

Usage

```
rTimeOutliers(
  object,
  leftRT = "leftRT",
  rightRT = "rightRT",
  searchRT = "Search.RT"
)
```

Arguments

object	An object of class QFeatures
leftRT	A character indicated pattern associated with left boundary of retention time search. Default is "leftRT".
rightRT	A character indicated pattern associated with right boundary of retneton time search. Default is "rightRT".
searchRT	The actual search retention time pattern. Default is "Search.RT"

Value

A list indicating the retention time based outliers.

Author(s)

Oliver Crook

Examples

```
data("BRD4df_full")

rTimeOutliers(BRD4df_full)
```

`spectraSimilarity` *Spectral checking using data from HDsite*

Description

Spectral checking using data from HDsite

Usage

```
spectraSimilarity(
  peaks,
  object,
  experiment = NULL,
  mzCol = 14,
  startRT = "Start.RT",
  endRT = "End.RT",
  charge = "z",
  incorpD = "X.D.left",
  maxD = "maxD",
  numSpectra = NULL,
  ppm = 300,
  BPPARAM = bpparam()
)
```

Arguments

`peaks`	a data.frame containing data exported from hdsite
`object`	a data.frame obtained from HDexaminer data
`experiment`	A character vector indicating the experimental conditions
`mzCol`	The column in the peak information indicating the base mz value
`startRT`	The column indicatng the start of the retention time. Default is "Start.RT"
`endRT`	The column indicating the end of the retention time. Default is "End.RT
`charge`	The column indicating the charge information. Default is "z".
`incorpD`	The deuterium uptake value column. Default is "X.D.left".
`maxD`	The maximum allowed deuterium incorporation column. Default is "maxD".

numSpectra	The number of spectra to analyse. Default is NULL in which all Spectra are analysed.
ppm	The ppm error
BPPARAM	Bioconductor parallel options.

Value

Two list of spectra observed and matching theoretical Spectra

Author(s)

Oliver Crook

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