# Package 'hdxmsqc'

January 24, 2026

**Type** Package

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

**Version** 1.7.0

**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.

**License** file LICENSE

**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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Metabolomics

**BugReports** https://github.com/ococrook/hdxmsqc/issues

**URL** http://github.com/ococrook/hdxmsqc

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# Contents

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| 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

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| | |
|---|---|
| `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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