

# Package ‘hdxmsqc’

August 10, 2025

**Type** Package

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

**Version** 1.4.0

**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 interactive 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

**Roxygen** list(markdown=TRUE)

**RoxygenNote** 7.2.3

**biocViews** QualityControl,DataImport, Proteomics, MassSpectrometry, Metabolomics

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

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

**Language** en-US

**git\_url** <https://git.bioconductor.org/packages/hdxmsqc>

**git\_branch** RELEASE\_3\_21

**git\_last\_commit** ee32357

**git\_last\_commit\_date** 2025-04-15

**Repository** Bioconductor 3.21

**Date/Publication** 2025-08-10  
**Author** Oliver M. Crook [aut, cre] (ORCID:  
    <<https://orcid.org/0000-0001-5669-8506>>)  
**Maintainer** Oliver M. Crook <oliver.crook@stats.ox.ac.uk>

**Contents**

|                                          |           |
|------------------------------------------|-----------|
| BRD4df . . . . .                         | 2         |
| BRD4df_full . . . . .                    | 3         |
| chargeCorrelationHdx . . . . .           | 3         |
| compatibleUptake . . . . .               | 4         |
| computeMassError . . . . .               | 4         |
| computeMonotoneStats . . . . .           | 5         |
| exchangeableAmides . . . . .             | 6         |
| fourierIsotope . . . . .                 | 6         |
| generateSpectra . . . . .                | 7         |
| hdxmsqc . . . . .                        | 8         |
| imTimeOutlier . . . . .                  | 8         |
| intensityOutliers . . . . .              | 9         |
| isMissingAtRandom . . . . .              | 10        |
| isotopicDistributionHDXfourier . . . . . | 10        |
| plotImTimeOutlier . . . . .              | 11        |
| plotIntensityOutliers . . . . .          | 12        |
| plotMassError . . . . .                  | 13        |
| plotMissing . . . . .                    | 13        |
| plotMonotoneStat . . . . .               | 14        |
| plotrTimeOutliers . . . . .              | 15        |
| processHDE . . . . .                     | 16        |
| qualityControl . . . . .                 | 16        |
| replicateCorrelation . . . . .           | 18        |
| replicateOutlier . . . . .               | 19        |
| rTimeOutliers . . . . .                  | 20        |
| spectraSimilarity . . . . .              | 21        |
| <b>Index</b>                             | <b>23</b> |

---

|        |                                                  |
|--------|--------------------------------------------------|
| BRD4df | <i>This is data to be included in my package</i> |
|--------|--------------------------------------------------|

---

**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 | <i>This is data to be included in my package</i> |
|-------------|--------------------------------------------------|

---

**Description**

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

**Author(s)**

My Name <ococrook@gmail.com>

---

|                      |                                                                                                 |
|----------------------|-------------------------------------------------------------------------------------------------|
| chargeCorrelationHdx | <i>Charge states should have correlated incorporation but they need not be exactly the same</i> |
|----------------------|-------------------------------------------------------------------------------------------------|

---

**Description**

Charge states should have correlated incorporation 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 | <i>Check whether deuterium uptakes are compatible with difference overlapping sequences.</i> |
|------------------|----------------------------------------------------------------------------------------------|

---

### 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 consistency. 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 | <i>Empirical versus theoretical mass errors</i> |
|------------------|-------------------------------------------------|

---

### 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 | <i>Compute exchangeable amides.</i> |
|--------------------|-------------------------------------|

---

**Description**

Computes the number of exchangeable amides based on the sequence

**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 | <i>fourier transform approach to computing isotopic distribution</i> |
|----------------|----------------------------------------------------------------------|

---

**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 incorporation                                                                                                                       |
| num_exch_sites | The number of exchangeable amides. Default is 0.                                                                                                  |
| charge         | The charge state of the peptide                                                                                                                   |
| isotopes       | The number of isotopes to compute. The default is NULL, in which 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 incorporation      |
| 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 | <i>A package to perform quality control for mass-spectrometry based hydrogen deuterium exchange experiment.</i> |
|---------|-----------------------------------------------------------------------------------------------------------------|

---

### 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 HDEaminer or DynamX software. There is not need to filter the data in either of those software systems.

### Author(s)

Oliver Crook

---

|               |                                                 |
|---------------|-------------------------------------------------|
| imTimeOutlier | <i>Ion Mobility time based outlier analysis</i> |
|---------------|-------------------------------------------------|

---

### 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 | <i>Intensity based deviations</i> |
|-------------------|-----------------------------------|

---

## 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 | <i>Missing at random versus missing not at random</i> |
|-------------------|-------------------------------------------------------|

---

**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 logical indicating whether to filter out data that is deemed missing not at random<br><pre>data("BRD4df_full") isMissingAtRandom(BRD4df_full)</pre>                               |

**Value**

Adds a missing not at random indicator column

**Author(s)**

Oliver Crook

---

|                                |                                                                      |
|--------------------------------|----------------------------------------------------------------------|
| isotopicDistributionHDXfourier | <i>fourier transform approach to computing isotopic distribution</i> |
|--------------------------------|----------------------------------------------------------------------|

---

**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 incorporation                                             |
| 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 | <i>Ion Mobility time based outlier analysis</i> |
|-------------------|-------------------------------------------------|

---

**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 | <i>Mass error plot</i> |
|---------------|------------------------|

---

**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 | <i>missing value plot</i> |
|-------------|---------------------------|

---

**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 | <i>Monotonicity based outlier detection, plot.</i> |
|------------------|----------------------------------------------------|

---

**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 | <i>Retention time based analysis</i> |
|-------------------|--------------------------------------|

---

## 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 retention 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 | <i>Function to curate and HDExaminer file so that it contains all the information in a sensible format. This object can then be straightforwardly passed to a object of class QFeatures</i> |
|------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|

---

### Description

Function to curate and HDExaminer file so that it 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 | <i>Quality Control table function. Generate a table that collates quality control metrics</i> |
|----------------|-----------------------------------------------------------------------------------------------|

---

### 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 spectraSimilarity 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 | <i>Correlation based checks</i> |
|------------------|---------------------------------|

---

**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 | <i>Retention time based analysis</i> |
|---------------|--------------------------------------|

---

**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 retention 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 | <i>Spectral checking using data from HDsite</i> |
|-------------------|-------------------------------------------------|

---

## 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

# Index

## \* data

BRD4df, [2](#)

BRD4df\_full, [3](#)

BRD4df, [2](#)

BRD4df\_full, [3](#)

chargeCorrelationHdx, [3](#)

compatibleUptake, [4](#)

computeMassError, [4](#)

computeMonotoneStats, [5](#)

exchangeableAmides, [6](#)

fourierIsotope, [6](#)

generateSpectra, [7](#)

hdxmsqc, [8](#)

imTimeOutlier, [8](#)

intensityOutliers, [9](#)

isMissingAtRandom, [10](#)

isotopicDistributionHDXfourier, [10](#)

plotImTimeOutlier, [11](#)

plotIntensityOutliers, [12](#)

plotMassError, [13](#)

plotMissing, [13](#)

plotMonotoneStat, [14](#)

plotrTimeOutliers, [15](#)

processHDE, [16](#)

qualityControl, [16](#)

replicateCorrelation, [18](#)

replicateOutlier, [19](#)

rTimeOutliers, [20](#)

spectraSimilarity, [21](#)