

# Package ‘hdxmsqc’

September 13, 2025

**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.

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

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---

|        |                                                  |
|--------|--------------------------------------------------|
| 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

*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 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 | <i>generate Spectra using a fourier transform</i> |
|-----------------|---------------------------------------------------|

---

**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 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 outliers

**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

*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 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

*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 | <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 HDEaminer 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</i> |
|------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|

---

**Description**

Function to curate and HDEaminer 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(HDEaminerFile, proteinStates = NULL)
```

**Arguments**

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

**Value**

A wide format data frame with HDEaminer data

**Author(s)**

Oliver Crook

**Examples**

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

|                                   |                                                                                 |
|-----------------------------------|---------------------------------------------------------------------------------|
| <code>object</code>               | An object of class <code>Qfeatures</code> , with the data used for the analysis |
| <code>massError</code>            | The output of the <code>computeMassError</code> function                        |
| <code>intensityOutlier</code>     | The output of the <code>intensityOutliers</code> function                       |
| <code>retentionOutlier</code>     | The output of the <code>rTimeOutliers</code> function                           |
| <code>monotonicityStat</code>     | The output of the <code>computeMonotoneStats</code> function                    |
| <code>mobilityOutlier</code>      | The output of the <code>imTimeOutliers</code> function                          |
| <code>chargeCorrelation</code>    | The output of the <code>chargeCorrelationsHdx</code> function                   |
| <code>replicateCorrelation</code> | The output of the <code>replicateCorrelation</code> function                    |
| <code>replicateOutlier</code>     | The output of the <code>replicateOutlier</code> function                        |
| <code>sequenceCheck</code>        | The output of the <code>compatibleUptake</code> function                        |
| <code>spectraCheck</code>         | The output of the <code>spectraSimiarity</code> function                        |
| <code>experiment</code>           | The experimental conditions.                                                    |
| <code>timepoints</code>           | The timepoints used in the analysis, must include repeat for replicates         |
| <code>undeuterated</code>         | 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 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)**

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