

# Package ‘binneR’

February 8, 2019

**Type** Package

**Title** Spectral Processing for High Resolution Flow Infusion Mass Spectrometry

**Version** 2.0.10

**Description** A spectral binning approach for high resolution flow infusion mass spectrometry data.

**URL** <https://github.com/aberHRML/binneR>

**Encoding** UTF-8

**Imports** dplyr, magrittr, mzR, plyr, tidyr, methods, purrr, stringr, tibble, crayon, cli, lubridate, ggplot2, ggthemes

**License** GPL (>= 3)

**RoxygenNote** 6.1.1

**Collate** 'allGenerics.R' 'allClasses.R' 'binneRlyse.R' 'binParameters.R' 'binPurity.R' 'binCentrality.R' 'spectralBinning-method.R' 'show-method.R' 'info-method.R' 'binnedData-method.R' 'accurateData-method.R' 'getPeaks.R' 'calcBinList.R' 'getHeaders.R' 'calcBinMeasures.R' 'combScans.R' 'readFiles.R' 'sampProcess.R' 'binneR.R' 'plotBin.R' 'detectInfusionScans.R' 'plotChromatogram.R' 'plotTIC.R'

**Suggests** knitr, rmarkdown, gridExtra, metaboData (>= 0.2.3), prettydoc, htmltools, covr, testthat, gifski

**VignetteBuilder** knitr

**Additional\_repositories** <https://aberhrml.github.io/drat/>

**NeedsCompilation** no

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**Repository** CRAN

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accurateData	<i>accurateData-Binalysis</i>
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### Description

Extract accurate data from a Binalysis object.

### Usage

```
accurateData(x)
```

```
## S4 method for signature 'Binalysis'
accurateData(x)
```

### Arguments

x                    Binalysis object

### Author(s)

Jasen Finch <jsf9@aber.ac.uk>

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Binalysis-class	<i>Binalysis</i>
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**Description**

An S4 class to store spectrally binned data and accurate mass information.

**Slots**

binLog date and time of initiation of spectral binning  
binParameters object of class BinParameters containing the parameters for spectral binning  
files file paths for raw data  
info tibble containing runinfo data  
binnedData list containing tibbles of spectrally binned data for each acquisition mode  
accurateMZ tibble containin accurate mass information  
spectra list containing tibbles of headers and class master mix fingerprints

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binnedData	<i>binnedData-Binalysis</i>
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**Description**

Extract binned data from a Binalysis object.

**Usage**

```
binnedData(x)  
  
## S4 method for signature 'Binalysis'  
binnedData(x)
```

**Arguments**

x Binalysis object

**Author(s)**

Jasen Finch <jsf9@aber.ac.uk>

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binneRlyse

*binneRlyse*


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### Description

perform spectral binning.

### Usage

```
binneRlyse(files, info, parameters = binParameters(), verbose = T)
```

### Arguments

files	character vector of file paths to use for spectral binning
info	tibble containing sample information
parameters	object of class BinParameters containing parameters for spectral binning
verbose	show console output

### Examples

```
## Not run:
files <- metaboData::filePaths('FIE-HRMS', 'BdistachyonEcotypes')

info <- metaboData::runinfo('FIE-HRMS', 'BdistachyonEcotypes')

analysis <- binneRlyse(files,
                       info,
                       parameters = binParameters(detectInfusionScans(files)))

## End(Not run)
```

---

binParameters

*binParameters*


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### Description

selection of parameters to use for spectral binning.

### Usage

```
binParameters(scans = 5:12, modes = c("n", "p"), sranges = list(c(70,
1000)), cls = character(), nCores = detectCores(),
clusterType = "FORK")
```

**Arguments**

scans	numeric vector containing the scan indexes to use for binning
modes	character vector denoting the order and names of the modes
sranges	list of vectors containing the ranges of the scan events present
cls	the column of class labels to use for aggregating accurate mass data. Defaults to NULL where accurate mass data will be averaged accross all samples
nCores	the number of cores to use for parallel processing
clusterType	the type of cluster to use for parallel processing

**Examples**

```
p <- binParameters(scans = 6:17,nCores = 2,clusterType = 'PSOCK')

## Example using multiple overlapping scan ranges
p <- binParameters(scans = 6:17,sranges = list(c(55,280),c(270,1200)))
```

---

BinParameters-class    *BinParameters*

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**Description**

An S4 class to store spectral binning parameters.

**Slots**

scans	numeric vector containing the scan indexes to use for binning
modes	character vector denoting the order and names of the modes
sranges	list of vectors containing the ranges of the scan events present
cls	the column of class labels to use for aggregating accurate mass data. Defaults to NULL where accurate mass data will be averaged accross all samples
nCores	the number of cores to use for parallel processing
clusterType	the type of cluster to use for parallel processing

detectInfusionScans    *detectInfusionScans*

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### Description

detect infusion scans for a set of FIE-MS infusion profiles.

### Usage

```
detectInfusionScans(files, sranges = list(c(70, 1000)), thresh = 0.5)
```

### Arguments

files	character vector of file paths to use
sranges	A list of vectors containing the scan events present.
thresh	detection threshold as a proportion of peak of the infusion profile

### Examples

```
if (requireNamespace("metaboData", quietly = TRUE)) {  
  detectInfusionScans(metaboData::filePaths('FIE-HRMS', 'BdistachyonEcotypes')[1])  
}
```

---

info                    *info-Binalysis*

---

### Description

Extract runinfo data from a Binalysis object.

### Usage

```
info(x)  
  
## S4 method for signature 'Binalysis'  
info(x)
```

### Arguments

x	Binalysis object
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### Author(s)

Jasen Finch <jsf9@aber.ac.uk>

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plotBin	<i>plotBin</i>
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**Description**

kernal density plot of a specified bin.

**Usage**

```
plotBin(x, bin, cls = T)
```

```
## S4 method for signature 'Binalysis'  
plotBin(x, bin, cls = T)
```

**Arguments**

x	S4 object of class Binalysis
bin	0.01amu bin to plot
cls	TRUE or FALSE. Should bins be plotted by class?

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plotChromatogram	<i>plotChromatogram</i>
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**Description**

plot an averaged infusion profile from a Binalysis object.

**Usage**

```
plotChromatogram(x)
```

```
## S4 method for signature 'Binalysis'  
plotChromatogram(x)
```

**Arguments**

x	S4 object of class Binalysis
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plotChromFromFile      *plotChromFromFile*

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**Description**

plot and averaged infusion profile from a vector of specified file paths.

**Usage**

```
plotChromFromFile(files, sranges = list(c(70, 1000)), scans = c())
```

**Arguments**

files	character vector of file paths to use
sranges	A list of vectors containing the scan events present
scans	specify scans to highlight within the plot

**Examples**

```
plotChromFromFile(list.files(system.file('mzML', package = 'binneR'),  
                             full.names=TRUE), scans = c(6,18))
```

---

plotTIC      *plotTIC*

---

**Description**

Plot sample total ion counts.

**Usage**

```
plotTIC(x, by = "injOrder", colour = "block")  
  
## S4 method for signature 'Binalysis'  
plotTIC(x, by = "injOrder", colour = "block")
```

**Arguments**

x	S4 object of class Binalysis
by	info column to plot against
colour	info column to provide colour labels



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readFiles	<i>Read and process multiple data files</i>
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**Description**

Apply spectral binning on multiple data files.

**Usage**

```
readFiles(files, dp, scans, sranges = list(c(50, 1000)), modes = c("n",  
  "p"), nCores = 1)
```

**Arguments**

files	A vector of converted data file paths
dp	An integer denoting the number of decimal places for spectral binning
scans	A vector of scan numbers that should be retrieved
sranges	A list of vectors containing the scan events present.
modes	A vector of strings denoting mode names including the order in which the scan events occur.
nCores	The number of cores on which to parallel process.

**Value**

A list containing peak lists for the relevant scans with combined scan ranges for each present mode in the data file.

**Author(s)**

Jasen Finch

**Examples**

```
res <- readFiles(list.files(system.file('mzML', package = 'binner'),  
  full.names=TRUE), dp = 2, scans = 6:17)
```

show, Binalysis-method *show-Binalysis*

---

**Description**

show method for Binalysis class

**Usage**

```
## S4 method for signature 'Binalysis'  
show(object)
```

**Arguments**

object            Binalysis Object

**Author(s)**

Jasen Finch <jsf9@aber.ac.uk>

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show, BinParameters-method  
*show-BinParameters*

---

**Description**

show method for BinParameters class

**Usage**

```
## S4 method for signature 'BinParameters'  
show(object)
```

**Arguments**

object            BinParameters Object

**Author(s)**

Jasen Finch <jsf9@aber.ac.uk>

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