Package 'binneR'

January 16, 2019

Type Package

Title Spectral Processing for High Resolution Flow Infusion Mass Spectrometry

Version 2.0.7

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

URL https://github.com/jasenfinch/binneR

Encoding UTF-8

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

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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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R topics documented:

`accurateData` *accurateData-Binalysis*

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>

Binalysis-class *Binalysis*

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

binnedData *binnedData-Binalysis*

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>

binneRlyse *binneRlyse*

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*

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

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BinParameters-class *BinParameters*

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

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detectInfusionScans *detectInfusionScans*

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 preak 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

Author(s)

Jasen Finch <jsf9@aber.ac.uk>

`plotBin` *plotBin*

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?

plotChromatogram *plotChromatogram*

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

plotChromFromFile *plotChromFromFile*

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

readFiles *Read and process mulitple data files*

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)
```

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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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