Package: binneR (via r-universe)

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Title Spectral Processing for High Resolution Flow Infusion Mass Spectrometry

Version 2.6.4

Description A spectral binning approach for flow infusion electrospray high resolution mass spectrometry (FIE-HRMS) metabolome fingerprinting data. The methodology for this approach is outlined in Finch et al. (2022) <doi:10.1007/s11306-022-01923-6>.

biocViews MassSpectrometry, Metabolomics

URL `https://aberhrml.github.io/binneR/`, `http://aberhrml.github.io/binneR/`

BugReports `https://github.com/aberHRML/binneR/issues`

Depends R (>= 3.5)

Imports dplyr, magrittr, mzR, tidyr, methods, purrr, stringr, tibble, crayon, cli, lubridate, ggplot2, ggthemes, yaml, future, furrr

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Contents

`Binalysis-class` *Spectral binning analysis class*

Description

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

Slots

`version` package version

`creation_date` creation date

`file_paths` file paths for raw data

`sample_info` tibble containing runinfo data

`binned_data` list containing tibbles of spectrally binned data for each acquisition mode

`accurate_mz` tibble containin accurate mass information

`spectra` list containing tibbles of headers and class master mix fingerprints

See Also

`binneRlyse`

`binneRlyse` *Perform spectral binning*

Description

perform spectral binning.

Usage

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

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

Details

Parallel processing is managed by the `future` package. This can be specified using the `plan()` `function`. See the example below and `?future::plan` for details on how this can be specified.

By default, spectral binning is performed at the recommended 2 decimal places. This can be altered by setting either the global option `binner_dp` or the environment variable `BINNER_DP`.

Value

S4 object of class Binalysis.

See Also

`Binalysis-class`, `binParameters`, `sampleInfo`, `binnedData`, `accurateData`

Examples

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

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

parameters <- detectParameters(files)
cls(parameters) <- 'class'

## Optionally declare parallel processing backend
# plan(future::multisession,workers = 2)

analysis <- binneRlyse(files,
                       info,
```

```
                                parameters = parameters)

## End(Not run)
```

`binParameters` *Set spectral binning parameters*

Description

Selection of parameters to use for spectral binning.

Usage

```
binParameters(scans = 5:12, cls = character())
```

Arguments

`scans`	numeric vector containing the scan indexes to use for binning
`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

Value

S4 object of class BinParameters

See Also

`BinParameters-class`, `scans`, `cls`

Examples

```
p <- binParameters(scans = 6:17)
```

`BinParameters-class` *Spectral binning parameters class*

Description

An S4 class to store spectral binning parameters.

Slots

`scans` numeric vector containing the scan indexes to use for binning

`cls` the column of class labels to use for aggregating accurate mass data. Defaults to NULL where accurate mass data will be averaged across all samples

See Also

`binParameters`

`detectInfusionScans` *Detect infusion profile scan range*

Description

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

Usage

```
detectInfusionScans(files, thresh = 0.5)
```

Arguments

`files`	character vector of file paths to use
`thresh`	detection threshold as a proportion of the peak of the infusion profile

Value

Numeric vector of detected infusion scans.

See Also

`detectParameters`

Examples

```
file_paths <- system.file('example-data/1.mzML.gz',package = 'binneR')

detectInfusionScans(file_paths)
```

`detectParameters` *Detect suitable spectral binning parameters*

Description

Detect binning parameters from a given list of file paths.

Usage

```
detectParameters(files)
```

Arguments

`files`	character vector of file paths

Value

S4 object of class BinParameters

See Also

`BinParameters-class`, `binParameters`

Examples

```
file_paths <-system.file('example-data/1.mzML.gz',package = 'binneR')
parameters <- detectParameters(file_paths)
```

`plotBin` *Plot a spectral bin feature*

Description

Kernal density plot of a specified spectral bin feature.

Usage

```
plotBin(x, bin, type = c("all", "cls", "sample"))

## S4 method for signature 'Binalysis'
plotBin(x, bin, type = c("all", "cls", "sample"))
```

Arguments

`x`	S4 object of class Binalysis
`bin`	0.01amu bin to plot
`type`	bin to be plotted as a total (all), class (cls) or sample spectra.

See Also

`accurateData`, `binneRlyse`

`plotCentrality` *Plot bin centrality histogram*

Description

Plot the bin centrality distribution for a Binalysis object.

Usage

```
plotCentrality(x, histBins = 30)

## S4 method for signature 'Binalysis'
plotCentrality(x, histBins = 30)
```

Arguments

`x`	S4 object of class Binalysis
`histBins`	number of bins to use for histogram plotting

See Also

`accurateData`, `binneRlyse`, `plotPurity`

`plotChromatogram` *Plot an infusion profile chromatogram*

Description

Plot an averaged infusion profile chromatogram from a Binalysis object.

Usage

```
plotChromatogram(x)

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

Arguments

`x`	S4 object of class `Binalysis`

See Also

`binneRlyse`

`plotChromFromFile` *Plot an infusion profile chromatogram from a file*

Description

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

Usage

```
plotChromFromFile(files, scans = c())
```

Arguments

`files`	character vector of file paths to use
`scans`	specify scans to highlight within the plot

Examples

```
file_paths <- system.file('example-data/1.mzML.gz',package = 'binneR')

plotChromFromFile(file_paths,
                  scans = detectInfusionScans(file_paths))
```

`plotFingerprint` *Plot a fingerprint mass spectrum*

Description

Plot averaged spectrum fingerprint.

Usage

```
plotFingerprint(x)

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

Arguments

`x`	S4 object of class Binalysis

See Also

`binneRlyse`

`plotPurity` *Plot bin purity histogram*

Description

Plot the bin purity distribution for a Binalysis object.

Usage

```
plotPurity(x, histBins = 30)

## S4 method for signature 'Binalysis'
plotPurity(x, histBins = 30)
```

Arguments

`x`	S4 object of class Binalysis
`histBins`	number of bins to use for histogram plotting

See Also

`accurateData`, `binneRlyse`, `plotCentrality`

`plotTIC` *Plot sample total ion counts*

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

See Also

`binneRlyse`

`readBinningParameters` *Read binning parameters from file*

Description

Parse binning parameters from a YAML formatted file.

Usage

```
readBinningParameters(file)
```

Arguments

`file`	file path

Value

S4 object of class BinParameters.

See Also

`BinParameters-class`

Examples

```
file <- system.file('binning_parameters.yml',package = 'binneR')
parameters <- readBinningParameters(file)
```

`readFiles` *Read and process mulitple data files*

Description

Apply spectral binning on multiple data files.

Usage

```
readFiles(files, dp, scans)
```

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

Details

Parallel processing is managed by the `future` package. This can be specified using the `plan()` `function`. See the example below and `?future::plan` for details on how this can be specified.

Value

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

Examples

```
## Example file path
file_paths <- system.file('example-data/1.mzML.gz',package = 'binneR')

## Optionally declare parallel processing backend
# plan(future::multisession,workers = 2)

## Process example file
res <- readFiles(file_paths,
                 dp = 2,
                 scans = detectInfusionScans(file_paths))
```

`scans` *Get and set spectral binning parameters*

Description

Get and set spectral binning parameters.

Usage

```
scans(x)

scans(x) <- value

cls(x)

cls(x) <- value

## S4 method for signature 'BinParameters'
scans(x)

## S4 replacement method for signature 'BinParameters'
scans(x) <- value

## S4 method for signature 'BinParameters'
cls(x)
```

```
## S4 replacement method for signature 'BinParameters'
cls(x) <- value
```

Arguments

`x`	S4 object of class BinParameters
`value`	parameter value to set

See Also

`BinParameters-class`, `binParameters`

`show,BinParameters-method`

Show methods for spectral binning classes

Description

Show methods for spectral binning classes.

Usage

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

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

Arguments

`object`	S4 objects of class BinParameters or Binanalysi

Author(s)

Jasen Finch <`jsf9@aber.ac.uk`>

`singleSample` *Perform single sample spectral binning*

Description

Perform spectral binning on a single sample.

Usage

```
singleSample(file, class = NA, verbose = TRUE)
```

Arguments

`file`	file path
`class`	optional class name
`verbose`	show console output

Details

Parallel processing is managed by the `future` package. This can be specified using the `plan()` `function`. See the example below and `?future::plan` for details on how this can be specified.

By default, spectral binning is performed at the recommended 2 decimal places. This can be altered by setting either the global option `binner_dp` or the environment variable `BINNER_DP`.

Value

S4 object of class Binalysis.

See Also

`Binalysis-class`

Examples

```
## Not run:
file_path <- metaboData::filePaths('FIE-HRMS','BdistachyonTechnical')[1]

## Optionally declare parallel processing backend
# plan(future::multisession,workers = 2)

bd <- singleSample(file_path)

## End(Not run)
```

`version` *Binalysis class get methods*

Description

Methods for accessing spectral binning results from the Binalysis S4 class.

Usage

```
version(x)

creationDate(x)

filePaths(x)

sampleInfo(x)

binnedData(x)

accurateData(x)

binningParameters(x)

## S4 method for signature 'Binalysis'
version(x)

## S4 method for signature 'Binalysis'
creationDate(x)

## S4 method for signature 'Binalysis'
filePaths(x)

## S4 method for signature 'Binalysis'
sampleInfo(x)

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

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

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

Arguments

`x`	S4 object of class Binalysis

Details

- version - Extract package version used to create the object.
- creationDate - Extract the creation date of the object.
- filePaths - Extract the sample file paths.
- sampleInfo - Extract sample meta information.
- binnedData - Extract a binned data intensity matrix.
- accurateData - Extract sample-wise accurate mass data and bin measures.
- binningParametesrExtract the binning parameters.

See Also

`Binalysis-class`, `binneRlyse`

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