Package: sRm (via r-universe)

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Type Package

Title Toolkit for SRM-MS data (MS) data

Version 0.2.6

Description A complete toolkit for working with Selective Reaction Monitoring (SRM) Mass Spectrometry (MS) data and other variants of targeted Liquid Chromatography (LC) MS data.

License GPL (>= 3)

Depends ggplot2, magrittr

Imports methods, MSnbase, tibble, purrr, dplyr, tidyr, xml2, xcms, stringr, MsCoreUtils, cli, crayon, furrr, future

URL https://github.com/wilsontom/sRm

BugReports https://github.com/wilsontom/sRm/issues

LazyData TRUE

Encoding UTF-8

RoxygenNote 7.2.3

Suggests testthat, knitr, rmarkdown, patchwork

Roxygen list(markdown = TRUE)

VignetteBuilder knitr

Collate 'allGenerics.R' 'allClasses.R' 'accessor-method.R' 'adjustBaseline-method.R' 'createGroup-method.R' 'detectInstrumentModel.R' 'detectPeaks-method.R' 'fileMetaData.R' 'filterPeaks-method.R' 'freeScales.R' 'groupPeaks-method.R' 'groupSummary-method.R' 'indexRT-method.R' 'internals.R' 'keepTransitions-method.R' 'openSRM.R' 'peakAsymmetry-method.R' 'plotGroup-method.R' 'plotParent-method.R' 'plotPeakArea-method.R' 'plotSRM-method.R' 'plotSample-method.R' 'reducePeaks-method.R' 'removeSample-method.R' 'removeTransitions-method.R' 'show-method.R' 'smoothChrom-method.R'

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Contents

`adjustBaseline` *Adjust Baseline*

Description

Adjust Baseline

Usage

```
adjustBaseline(object, hwm)

## S4 method for signature 'SRM'
adjustBaseline(object, hwm = 6)
```

Arguments

`object`	a SRM object
`hwm`	a numeric value for window half width for local medians

Value

a SRM object

`createGroup` *Create Group*

Description

Create peak group based on user specified retention time

Usage

```
createGroup(object, index, rt, width, id)

## S4 method for signature 'SRM'
createGroup(object, index, rt, width, id)
```

Arguments

`object`	a SRM object
`index`	a numeric value of the target transition index
`rt`	a numeric value of target Rt time (in minutes)
`width`	a numeric value of tolerated Rt width (in seconds)
`id`	a character string for peak group identification

Value

a `SRM` object

`detectInstrumentModel` *Detect Instrument Model*

Description

Detect Instrument Model

Usage

```
detectInstrumentModel(mzml_file)
```

Arguments

`mzml_file`	the absolute file path of a valid `.mzML` file

Value

a character string of the MS cvParam description for the instrument model

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`detectPeaks` *Detect Peaks*

Description

Detect Peaks

Usage

```
detectPeaks(object, snthresh, peakwidth)

## S4 method for signature 'SRM'
detectPeaks(object, snthresh, peakwidth)
```

Arguments

`object`	a SRM object
`snthresh`	a numeric value for the signal-to-noise threshold to use
`peakwidth`	a numeric vector indicating the minimum and maximum tolerated peak width

Value

a SRM object

`fileMetaData` *Extract meta information from .mzML file*

Description

Extract a minimal amount meta data from a `.mzML` file

Usage

```
fileMetaData(x)
```

Arguments

`x`	a valid `.mzML` file

Value

a `tibble` containing;

- mzML Schema
- Acquisition Date
- Acquisition Time
- Instrument Model
- File ID

`filterPeaks` *Filter Peaks*

Description

Filter detected peaks based on a series of heuristic measures

Usage

```
filterPeaks(object)

## S4 method for signature 'SRM'
filterPeaks(object)
```

Arguments

`object`	a SRM object

Value

a `SRM` object

`freeScales` *Free Scales*

Description

Allow `free` scales in facet plots

Usage

```
freeScales(ggplot)
```

Arguments

`ggplot`	a `ggplot` object

Value

a `ggplot` object

`groupPeaks` *Group Peaks*

Description

Group detected peaks based on retention time. Based on `MsCoreUtils::group`

Usage

```
groupPeaks(object, rt_tolerance)

## S4 method for signature 'SRM'
groupPeaks(object, rt_tolerance)
```

Arguments

`object`	a SRM object
`rt_tolerance`	a numeric value for the tolerate retention grouping

Value

a `SRM` object

`groupSummary` *Group Summary*

Description

Create a summary table for peak groups

Usage

```
groupSummary(object)

## S4 method for signature 'SRM'
groupSummary(object)
```

Arguments

`object`	a `SRM` object

Value

a `tibble` of group summary

`header` *header*

Description

List object header information

Usage

```
header(object)

## S4 method for signature 'SRM'
header(object)
```

Arguments

`object`	a `SRM` S4 object

`indexRT` *Find Target Retention Time (Rt) for a transition*

Description

Find Target Retention Time (Rt) for a transition

Usage

```
indexRT(object, index, sampleName, n)

## S4 method for signature 'SRM'
indexRT(object, index, sampleName, n = 1)
```

Arguments

`object`	a SRM object
`index`	a numeric value for the transition index
`sampleName`	a character string
`n`	a numeric value for the number of Rts to return (if > 1 is available)

Value

a numeric vector or Rt targets

`keepTransitions` *Keep Transitions*

Description

Keep Transitions

Usage

```
keepTransitions(object, index_keep)

## S4 method for signature 'SRM'
keepTransitions(object, index_keep = c())
```

Arguments

`object`	a SRM object
`index_keep`	a numeric vector of transition index to retain

Value

a `SRM` object

`meta` *meta*

Description

List sample meta data

Usage

```
meta(object)

## S4 method for signature 'SRM'
meta(object)
```

Arguments

`object`	a `SRM` S4 object

`openSRM` *Open SRM Files*

Description

Open and parse SRM files into an `S4` SRM Object

Usage

```
openSRM(files)
```

Arguments

`files`	a character vector of absolute file paths of SRM files in `.mzML` format

Value

an SRM object

`peakAsymmetry` *Peak Asymmetry*

Description

Peak Asymmetry

Usage

```
peakAsymmetry(object)

## S4 method for signature 'SRM'
peakAsymmetry(object)
```

Arguments

`object`	a SRM object

Value

a `SRM` object

`peaks` *peaks*

Description

List detected peaks

Usage

```
peaks(object)

## S4 method for signature 'SRM'
peaks(object)
```

Arguments

`object`	a `SRM` S4 object

`plotGroup` *Plot Group*

Description

Plot Group

Usage

```
plotGroup(object, group)

## S4 method for signature 'SRM'
plotGroup(object, group)
```

Arguments

`object`	a SRM object
`group`	a character string of the `GroupID`

Value

a ggplot plot object

`plotParent` *Plot Parent*

Description

Plot Parent

Usage

```
plotParent(object, parentMass)

## S4 method for signature 'SRM'
plotParent(object, parentMass)
```

Arguments

`object`	a SRM object
`parentMass`	a numeric value of the parent mass (Q1) to extract

Value

a ggplot plot object

`plotPeakArea` *Plot Peak Area*

Description

Plot Peak Area

Usage

```
plotPeakArea(object, index, sampleName)

## S4 method for signature 'SRM'
plotPeakArea(object, index, sampleName)
```

Arguments

`object`	a SRM object
`index`	a numeric value of the transition index to plot
`sampleName`	a character string of `sampleName` to plot

Value

a ggplot plot object

`plotSample` *Plot Sample*

Description

Plot Sample

Usage

```
plotSample(object, sampleName, polarity)

## S4 method for signature 'SRM'
plotSample(object, sampleName, polarity)
```

Arguments

`object`	a SRM object
`sampleName`	a character string of a valid `sampleName`
`polarity`	a character string of either `pos` or `neg` for positive and negative ionisation mode respectively

Value

a ggplot plot object

`plotSRM` *Plot SRM*

Description

Plot SRM

Usage

```
plotSRM(object, index, type = "overlay")

## S4 method for signature 'SRM'
plotSRM(object, index, type = "overlay")
```

Arguments

`object`	a SRM object
`index`	a numeric value of the transition index to plot
`type`	a character string of either `overlay` or `facet`

Value

a ggplot plot object

`reducePeaks` *Reduce Peaks*

Description

Reduce detected peaks using a relative area threshold

Usage

```
reducePeaks(object, relative_area)

## S4 method for signature 'SRM'
reducePeaks(object, relative_area = 0.05)
```

Arguments

`object`	a SRM object
`relative_area`	a numeric value between 0 and 1, for the threshold of relative peak area

Value

a `SRM` object

`removeSample` *Remove Sample*

Description

Remove Sample

Usage

```
removeSample(object, sampleName)

## S4 method for signature 'SRM'
removeSample(object, sampleName)
```

Arguments

`object`	a SRM object
`sampleName`	a character string of a `sampleName` to remove

Value

a `SRM` object

`removeTransitions` *Keep Transitions*

Description

Keep Transitions

Usage

```
removeTransitions(object, index_out)

## S4 method for signature 'SRM'
removeTransitions(object, index_out = c())
```

Arguments

`object`	a SRM object
`index_keep`	a numeric vector of transition index to remove

Value

a `SRM` object

`show,SRM-method` *show-SRM*

Description

show-SRM

Usage

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

Arguments

`object`	a SRM object

`smoothChrom` *Smooth Chromatograms*

Description

Smooth Chromatograms

Usage

```
smoothChrom(object, cf)

## S4 method for signature 'SRM'
smoothChrom(object, cf)
```

Arguments

`object`	a SRM object
`cf`	matrix, a coefficient matrix generated by MsCoreUtils::coefMA or MsCoreUtils::coefWMA

Value

a SRM object

`SRM-class` *SRM*

Description

A S4 class to store single reaction monitoring (SRM) mass spectrometry (MS) data

Slots

`meta` a `tibble` of a minimal amount of meta data.

`transitions` a `tibble` of all transitions names

`chroms` a `tibble` of retention time (rt) and intensity (int) values for all imported SRM chromatograms

`peaks` a `tibble` of detected peaks

`groups` a `tibble` of peak information for user defined groups

`header` a `tibble` of formatted header data from `mzR::header()`

`transitions` *Accessor Methods for the SRM S4 class*

Description

List all transitions

Usage

```
transitions(object)

## S4 method for signature 'SRM'
transitions(object)
```

Arguments

`object`	a `SRM` S4 object

Index