Package 'sRm'

May 24, 2021

Type Package

Title Toolkit for SRM-MS data
(MS) data

Version 0.2.1

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

License GPL (>= 3)

Depends ggplot2,
magrittr

Imports methods,
mzR,
tibble,
purrr,
dplyr,
tidyr,
xml2,
xcms,
stringr,
MsCoreUtils,
ptw,
cli,
crayon

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

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

LazyData TRUE

Encoding UTF-8

RoxygenNote 7.1.1

Suggests testthat,
knitr,
rmarkdown,
patchwork

Roxygen list(markdown = TRUE)

VignetteBuilder knitr

Collate 'allGenerics.R'
'allClasses.R'
'accessor-method.R'
'centWave.R'
'chromTransform-method.R'
'detectPeaks-method.R'
'filterPeaks-method.R'
'freeScales.R'
'get_meta.R'
'groupPeaks-method.R'
'groupSummary-method.R'
'internals.R'
'openSRM.R'
'peakAsymmetry-method.R'
'plotGroup-method.R'
'plotParent-method.R'
'plotPeakArea-method.R'
'plotSRM-method.R'
'plotSample-method.R'
'show-method.R'

R **topics documented:**

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centWave *Wraper for xcms centWave peak detection*

Description

Wraper for xcms centWave peak detection

Usage

```
centWave(rt, int, snthresh, peakwidth)
```

Arguments

rt	a numeric vector of chromatogram retention time in minutes
int	a numeric vector of chromatogram intensity
snthresh	a numeric value for the Signal-to-Noise cut off to use during peak detection
peakwidth	a numeric value for the minimum and maximum tolerated peak width.

Value

a `tibble` of detected peaks

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chromTransform *Transform Chromatograms*

Description

Transform Chromatograms

Usage

```
chromTransform(object, cf)

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

Arguments

object	a SRM object
cf	matrix, a coefficient matrix generated by MsCoreUtils::coefMA or MsCore-Utils::coefWMA

Value

a SRM object

---

detectPeaks   *Detect Peaks*

Description

Detect Peaks

Usage

```
detectPeaks(object, snthresh, peakwidth)

## S4 method for signature 'SRM'
detectPeaks(object, snthresh = 10, peakwidth = 30)
```

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

---

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

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get_meta *Extract meta information from .mzML file*

Description

Extract a minimal amount meta data from a .mzML file

Usage

```
get_meta(x, type = "raw")
```

Arguments

x   a valid .mzML file

type   a character string of the original file format (raw or lcd)

Value

a tibble containing;

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

---

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

meta	*meta*

Description

List sample meta data

Usage

```
meta(object)

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

Arguments

object   a SRM S4 object

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openSRM   *Open SRM Files*

Description

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

Usage

```
openSRM(files, source_type)
```

Arguments

`files`	a character vector of absolute file paths of SRM files in `.mzML` format
`source_type`	a character string of the original file format (`raw` or `lcd`)

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

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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

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plotSRM   *Plot SRM*

Description

Plot SRM

Usage

```
plotSRM(object, index, type)

## 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

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show,SRM-method *show-SRM*

Description

show-SRM

Usage

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

Arguments

object   a SRM object

SRM-class *SRM*

Description

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

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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

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