

Package ‘sRm’

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Type Package

Title Toolkit for SRM-MS data
(MS) data

Version 0.2.2

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,
mzR,
tibble,
purrr,
dplyr,
tidyr,
xml2,
xcms,
stringr,
MsCoreUtils,
ptw,
cli,
crayon,
q3ML

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'

'createGroup-method.R'

'detectPeaks-method.R'

'filterPeaks-method.R'

'freeScales.R'

'get_meta.R'

'groupPeaks-method.R'

'groupSummary-method.R'

'indexRT-method.R'

'internals.R'

'openSRM.R'

'peakAsymmetry-method.R'

'plotGroup-method.R'

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'plotSRM-method.R'

'plotSample-method.R'

'show-method.R'

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centWave	<i>Wrapper for xcms centWave peak detection</i>
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Description

Wrapper 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

chromTransform	<i>Transform Chromatograms</i>
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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-Utills::coefWMA

Value

a SRM object

createGroup	<i>Create Group</i>
-------------	---------------------

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

detectPeaks	<i>Detect Peaks</i>
-------------	---------------------

Description

Detect Peaks

Usage

```
detectPeaks(object, snthresh, peakwidth)
```

```
## S4 method for signature 'SRM'
```

```
detectPeaks(object, snthresh = 10, peakwidth = c(2, 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	<i>Filter Peaks</i>
-------------	---------------------

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
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Value

a SRM object

freeScales	<i>Free Scales</i>
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Description

Allow free scales in facet plots

Usage

```
freeScales(ggplot)
```

Arguments

ggplot	a ggplot object
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Value

a ggplot object

get_meta	<i>Extract meta information from .mzML file</i>
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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	<i>Group Peaks</i>
------------	--------------------

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	<i>Group Summary</i>
--------------	----------------------

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	<i>header</i>
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Description

List object header information

Usage

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

Arguments

object a SRM S4 object

indexRT	<i>Find Target Retention Time (Rt) for a transition</i>
---------	---

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

meta	<i>meta</i>
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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, backend = "mzR")
```

Arguments

<code>files</code>	a character vector of absolute file paths of SRM files in .mzML format
<code>source_type</code>	a character string of the original file format (raw or lcd)
<code>backend</code>	a character string of either mzR (Default) or q3ML. q3ML should only be used as a backend for files which have been converted using a version of pwiz which is not supported by mzR,

Value

an SRM object

`peakAsymmetry`*Peak Asymmetry*

Description

Peak Asymmetry

Usage

```
peakAsymmetry(object)
```

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

Arguments

<code>object</code>	a SRM object
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Value

a SRM object

peaks	<i>peaks</i>
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Description

List detected peaks

Usage

```
peaks(object)

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

Arguments

object a SRM S4 object

plotGroup	<i>Plot Group</i>
-----------	-------------------

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	<i>Plot Parent</i>
------------	--------------------

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	<i>Plot Peak Area</i>
--------------	-----------------------

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	<i>Plot Sample</i>
------------	--------------------

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	<i>Plot SRM</i>
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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

show, SRM-method	<i>show-SRM</i>
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Description

show-SRM

Usage

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

Arguments

object a SRM object

SRM-class	<i>SRM</i>
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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	<i>Accessor Methods for the SRM S4 class</i>
-------------	--

Description

List all transitions

Usage

```
transitions(object)

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

Arguments

object a SRM S4 object

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