

Package ‘sRm’

December 13, 2021

Type Package

Title Toolkit for SRM-MS data
(MS) data

Version 0.2.4

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,
furry,
future

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

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

LazyData TRUE

Encoding UTF-8

RoxygenNote 7.1.2

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'
'keepTransitions-method.R'
'openSRM.R'
'peakAsymmetry-method.R'
'plotGroup-method.R'
'plotParent-method.R'
'plotPeakArea-method.R'
'plotSRM-method.R'
'plotSample-method.R'
'removeSample-method.R'
'show-method.R'

R topics documented:

centWave	3
chromTransform	4
createGroup	4
detectPeaks	5
filterPeaks	5
freeScales	6
get_meta	6
groupPeaks	7
groupSummary	7
header	8
indexRT	8
keepTransitions	9
meta	9
openSRM	10

<i>centWave</i>	3
peakAsymmetry	10
peaks	11
plotGroup	11
plotParent	12
plotPeakArea	12
plotSample	13
plotSRM	13
removeSample	14
show,SRM-method	14
SRM-class	15
transitions	15
Index	16

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

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>
----------------	--------------------------------

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

Detect Peaks

Description

Detect Peaks

Usage

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

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

```
detectPeaks(object, snthresh = 10, peakwidth = c(2, 30), parallel = FALSE)
```

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
parallel	logical; if TRUE then future_map is used for peak detection

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	<i>Free Scales</i>
------------	--------------------

Description

Allow free scales in facet plots

Usage

freeScales(ggplot)

Arguments

ggplot a ggplot object

Value

a ggplot object

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

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

<code>object</code>	a SRM object
<code>rt_tolerance</code>	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

<code>object</code>	a SRM object
---------------------	--------------

Value

a tibble of group summary

header	<i>header</i>
--------	---------------

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

keepTransitions	<i>Keep Transitions</i>
-----------------	-------------------------

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	<i>meta</i>
------	-------------

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, source_type, backend = "mzR", parallel = FALSE)
```

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,
<code>parallel</code>	logical; if TRUE then future_map is used for opening files

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
---------------------	--------------

Value

a SRM object

peaks	<i>peaks</i>
-------	--------------

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>
---------	-----------------

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

removeSample	<i>Remove Sample</i>
--------------	----------------------

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

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

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

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

centWave, [3](#)
chromTransform, [4](#)
chromTransform, SRM-method
 (chromTransform), [4](#)
createGroup, [4](#)
createGroup, SRM-method (createGroup), [4](#)

detectPeaks, [5](#)
detectPeaks, SRM-method (detectPeaks), [5](#)

filterPeaks, [5](#)
filterPeaks, SRM-method (filterPeaks), [5](#)
freeScales, [6](#)

get_meta, [6](#)
groupPeaks, [7](#)
groupPeaks, SRM-method (groupPeaks), [7](#)
groupSummary, [7](#)
groupSummary, SRM-method (groupSummary),
 [7](#)

header, [8](#)
header, SRM-method (header), [8](#)

indexRT, [8](#)
indexRT, SRM-method (indexRT), [8](#)

keepTransitions, [9](#)
keepTransitions, SRM-method
 (keepTransitions), [9](#)

meta, [9](#)
meta, SRM-method (meta), [9](#)

openSRM, [10](#)

peakAsymmetry, [10](#)
peakAsymmetry, SRM-method
 (peakAsymmetry), [10](#)
peaks, [11](#)
peaks, SRM-method (peaks), [11](#)

plotGroup, [11](#)
plotGroup, SRM-method (plotGroup), [11](#)
plotParent, [12](#)
plotParent, SRM-method (plotParent), [12](#)
plotPeakArea, [12](#)
plotPeakArea, SRM-method (plotPeakArea),
 [12](#)
plotSample, [13](#)
plotSample, SRM-method (plotSample), [13](#)
plotSRM, [13](#)
plotSRM, SRM-method (plotSRM), [13](#)

removeSample, [14](#)
removeSample, SRM-method (removeSample),
 [14](#)

show, SRM-method, [14](#)
SRM-class, [15](#)

transitions, [15](#)
transitions, SRM-method (transitions), [15](#)