

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, furr, 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'

Config/pak/sysreqs

cmake libgmp-dev make libicu-dev libuv1-dev libxml2-dev libnetcdf-dev libssl-dev zlib1g-dev

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adjustBaseline	<i>Adjust Baseline</i>
----------------	------------------------

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	<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

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

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

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	<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

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

<code>groupSummary</code>	<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

<code>header</code>	<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

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

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	<i>Peak Asymmetry</i>
---------------	-----------------------

Description

Peak Asymmetry

Usage

```
peakAsymmetry(object)
```

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

Arguments

object a SRM object

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>
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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>
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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

reducePeaks	<i>Reduce Peaks</i>
-------------	---------------------

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	<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

removeTransitions	<i>Keep Transitions</i>
-------------------	-------------------------

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	<i>show-SRM</i>
------------------	-----------------

Description

show-SRM

Usage

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

Arguments

object a SRM object

smoothChrom	<i>Smooth Chromatograms</i>
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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 MsCore-
 Utils::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

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