Package 'sRm'

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Type Package

Title Minimal parser for Selective Reaction Monitoring (SRM) mass spectrometry (MS) data

Version 0.1.2

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Description Functions for parsing SRM-MS data from .mzML files.

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Depends methods, xml2 (>= 1.0), ggplot2, grid, gridExtra

Imports ggrepel, base64enc, Rcpp, gtable, scales, munsell, colorspace, plyr

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

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

LazyData TRUE

RoxygenNote 5.0.0

Suggests testthat

NeedsCompilation no

R topics documented:

combineTransitions *Combine Transitions*

Description

Combine Transitions

Each parent m/z will usually have multiple separate Q3 product ions. SRM transitions are stored separately in the mzML file. Each index is a transition from a single Q1 precursor ion to one of the specified Q3 ions. This method combines all Q3 product ion chromatograms into one, to produce a total ion chromatogram based on the parent m/z and all Q3 product ions assigned to that parent m/z

Usage

```
combineTransitions(object)

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

Arguments

object	a SRM object

Value

a transition class of SRM total ion chromatograms

Author(s)

Tom Wilson <tpw2@aber.ac.uk>

meta *Show meta data*

Description

Show meta data

Usage

```
meta(object)

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

Arguments

object	a SRM object

Author(s)

Tom Wilson <tpw2@aber.ac.uk>

`openSRMfile` *Open a SRM-MS file*

Description

Open and parse `mzML` file into `SRM` object

Usage

```
openSRMfile(filename)
```

Arguments

`filename`	a `mzML` file

Value

a `SRM` object (see `SRM-class`)

Author(s)

Tom Wilson <tpw2@aber.ac.uk>

`plotAll` *Plot all*

Description

Plot the SRM-MS TIC and all individual Q3 traces for a selected parent scans'

Usage

```
plotAll(x, n)

## S3 method for class 'transition'
plotAll(x, n)
```

Arguments

`x`	a `transition` class
`n`	the number of the transition (index) to plot

Author(s)

Tom Wilson <tpw2@aber.ac.uk>

plotMulti *plotMulti*

Description

plotMulti

Usage

```
plotMulti(object, idn)

## S4 method for signature 'SRM'
plotMulti(object, idn)
```

Arguments

object	a SRM object
idn	the index number of a transition to plot

Author(s)

Tom Wilson <tpw2@aber.ac.uk>

plotSRM *Plot SRM*

Description

Plot SRM

Usage

```
plotSRM(object, idn)

## S4 method for signature 'SRM'
plotSRM(object, idn)
```

Arguments

object	a SRM object
idn	the index number of a transition to plot

Author(s)

Tom Wilson <tpw2@aber.ac.uk>

show,SRM-method *show-SRM*

Description

show-SRM

Usage

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

Arguments

object	a SRM object

Author(s)

Tom Wilson <tpw2@aber.ac.uk>

SRM-class *SRM*

Description

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

Slots

env class environment

SHA1 character vector of the original SHA-1 checksum value

meta list containing file meta data

totalIonCount data.frame of sample total ion count (TIC)

index character vector of scan index's; ie SRM SIC 341.014,114.098

peaks list of peak data

header data.frame of summary information for each scan index; parentMz, Q3mz, totalIonCount, basePeakInt

`transitions` *Show transitions*

Description

Show transitions

Usage

```
transitions(object)

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

Arguments

`object`	a SRM object

Author(s)

Tom Wilson <tpw2@aber.ac.uk>

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