

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.

License GPL (>= 3)

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

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combineTransitions	<i>Combine Transitions</i>
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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
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Value

a transition class of SRM total ion chromatograms

Author(s)

Tom Wilson <tpw2@aber.ac.uk>

meta	<i>Show meta data</i>
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Description

Show meta data

Usage

```
meta(object)
```

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

Arguments

object	a SRM object
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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	<i>show-SRM</i>
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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	<i>SRM</i>
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Description

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

Slots

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	<i>Show transitions</i>
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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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