

Package ‘sRm’

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Type Package

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

Version 0.1.3

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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

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

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

LazyData TRUE

RoxygenNote 6.0.1

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

Where a dynamic MRM is used; then the start retention time (Rt) and end Rt is also taken into account when transitions are combined.

For example the following transitions from a standard SRM-MS experiment would be combined into a single chromatogram based on the parent m/z value;

- SRM SIC 153.01,65.271
- SRM SIC 153.01,67.232
- SRM SIC 153.01,109.094

Whereas the following transitions from a dynamic SRM-MS method would be combined into two different SRM TICs based on their parent m/z value and retention time window;

- SRM SIC Q1=145 Q3=56.996 start=10.61683333 end=20.84128333
- SRM SIC Q1=145 Q3=100.996 start=10.61665 end=20.84081667
- SRM SIC Q1=145 Q3=108.996 start=4.5304 end=10.53233333
- SRM SIC Q1=145 Q3=127.096 start=4.530016667 end=10.53213333

The above transitions would be combined to make the following;

Q1: 145 -> Q3: 56.996//100.996 (10.6 - 20.8)
Q1: 145 -> Q3: 108.996//127.096 (4.5 - 10.5)

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	<i>Plot all</i>
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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	<i>plotMulti</i>
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Description

plotMulti

Usage

```
plotMulti(object, idn, labels = NULL)

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

Arguments

object	a SRM object
idn	the index number of a transition to plot
labels	an optional character vector of label names. Default is NULL

Author(s)

Tom Wilson <tpw2@aber.ac.uk>

plotSRM	<i>Plot SRM</i>
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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
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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

SHA1 character vector of the original SHA-1 checksum value

meta list containing file meta data

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

filter character vector of scan filters; taken directly from chromatogram idRefs

index character vector of readable scan index's; ie Q1: 153.01 --> Q3: 65.271 (-)

peaks list of peak data

header data.frame of summary information for each scan index; parent, product, polarity, totIonCount, basePea

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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