Package 'sRm'

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Type Package

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

Version 0.1.4

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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, dplyr

Imports mzR (>= 2.1), ggrepel, tibble, purrr

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

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

LazyData TRUE

RoxygenNote 6.0.1

Suggests testthat

NeedsCompilation no

R topics documented:

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bpi   *bpi*

Description

bpi

Usage

```
bpi(object)

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

Arguments

```
object          a SRM object
```

Value

a numeric value for the whole sample base peak intensity (bpi)

Author(s)

Tom Wilson <tpw2@aber.ac.uk>

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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`

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
```

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>

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export_to_skyline	*export_to_skyline*

Description

export_to_skyline

Usage

```
export_to_skyline(object, transitions = NULL)

## S4 method for signature 'SRM'
export_to_skyline(object, transitions = NULL)
```

Arguments

```
object          a SRM object
```

```
transitions     an optional data.frame containing the following columns for selected (or all)
                transitions.
```

Value

a `tibble` of transitions in a format which can be easily used with `Skyline`

Author(s)

Tom Wilson <tpw2@aber.ac.uk>

---

get   *get*

Description

get

Usage

```
get(object, Q1, Q3, method)

## S4 method for signature 'SRM'
get(object, Q1, Q3, method)
```

Arguments

`object`	a SRM object
`Q1`	a numeric value for parent m/z
`Q3`	a numeric value for product m/z
`method`	either 'tic' or 'bpi' to return total ion count or base peak intensity respectively

Value

a `tibble` or parent and product mass, and either tic or bpi

---

get_meta   *Extract meta information from .mzML file*

Description

Extract a minimal amount meta data from a `.mzML` file

Usage

```
get_meta(x)
```

Arguments

`x`	a valid `.mzML` file

Value

a `tibble` containing;

- `mzML Schema`
- `Acquisition Date`
- `Acquisition Time`
- `Instrument Model`
- `File ID`

---

get_scan_header   *Extract scan header information*

Description

Extract key values (parent m/z, product m/z and polarity) from the `chromatogram` blocks of an `.mzML` file

Usage

```
get_scan_header(x)
```

Arguments

x   a valid `.mzML` file

Value

a `tibble` containing

- `header`
- `polarity`
- `Q1`
- `Q3`
- `tidy_head`

---

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>

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openSRMfile   *Open a SRM-MS file*

Description

Open and parse `mzML` file into a SRM object

Usage

```
openSRMfile(mzMLFile)
```

Arguments

mzMLFile   a valid .mzML file

Value

a SRM object (see [SRM-class](#))

Author(s)

Tom Wilson <tpw2@aber.ac.uk>

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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>

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plotMulti	*plotMulti*

Description

plotMulti

Usage

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

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

Arguments

object	a SRM object
idn	the index number of a transition to plot
addLabels	logical; If TRUE then labels for each geom_line are added
labels	an optional character vector of label names. Default is NULL. If addLabels is TRUE and labels is NULL then object@index is used for label text.

Author(s)

Tom Wilson <tpw2@aber.ac.uk>

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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>

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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

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, basePeakInt`

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tic   *tic*

Description

tic

Usage

```
tic(object)

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

Arguments

object   a SRM object

Value

a numeric value for the whole sample total ion count (tic)

Author(s)

Tom Wilson <tpw2@aber.ac.uk>

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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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