# 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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combineTransitions          *Combine Transitions*

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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
```

**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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get_meta                    *Extract meta information from .mzML file*

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## 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`

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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

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meta                                  *Show meta data*

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**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*

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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>

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plotMulti                  *plotMulti*

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## 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*

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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>

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SRM-class          *SRM*

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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

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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| transitions | *Show transitions* |
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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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