

Package ‘sRm’

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Type Package

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

Version 0.1.0

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Description Functions for parsing SRM-MS data stored in .mzML files.

License GPL (>= 3)

Depends methods, xml2 (>= 1.0)

Imports base64enc

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

BugReports <http://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

While each parent m/z will usually have three separate Q3 product ions, SRM transitions are stored separately in the mzML file. Each index is a single transition of parent m/z to one of the specified Q3 m/z 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 list 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

Author(s)

Tom Wilson <tpw2@aber.ac.uk>

openSRMfile *Open a SRM-MS file*

Description

Function for reading and parsing mzML file containing SRM-MS data

Usage

```
openSRMfile(filename)
```

Arguments

filename a mzML file

Value

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

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 file 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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