Package 'q3ML'

August 11, 2021

Type Package

Title Open and Parse SRM mzML files from Thermo Triple Quadruploe Mass Spectrometers

Version 0.1.0

Description More about what it does (maybe more than one line)
Use four spaces when indenting paragraphs within the Description.

License GPL (>= 3)

Encoding UTF-8

LazyData true

Depends magrittr

Imports xml2,
dplyr,
tidyr,
purrr,
tibble,
stringr,
base64enc,
crayon,
cli

RoxygenNote 7.1.1

Suggests covr,
testthat (>= 3.0.0),
mzR

Config/testthat/edition 3

Roxygen list(markdown = TRUE)

R topics documented:

decodePeaks *Decode peaks*

Description

Decode a binaryDataArray into a vector of either time or intensity

Usage

```
decodePeaks(x, compression = "none", size)
```

Arguments

x	a base64 encoded vector
compression	compression type (default = "none")
size	a numeric value for the number of bytes per element in the byte stream

Value

a numeric vector

idRefs *Extract mzML idRefs*

Description

Extract all the idRefs in the specified mzML file. The idRefs will correspond to the individual scan events.

Usage

```
idRefs(xmlDoc)
```

Arguments

xmlDoc	a xml document

Value

a character vector of all available idRefs

Examples

```
## Not run:
library(xml2)
xmlDoc <- read_xml("example_file.mzML")
xmlRefs <- idRefs(xmlDoc)
head(xmlRefs)
[1] "TIC"                      "SRM SIC 153.01,65.271"
[3] "SRM SIC 153.01,67.232"    "SRM SIC 153.01,109.094"
[5] "SRM SIC 179.022,107.007" "SRM SIC 179.022,134.006"

## End(Not run)
```

`openFile` *Open .mzML File*

Description

Open and parse a .mzML file containing Selective Reaction Monitoring (SRM) Mass Spectrometry (MS) data using `xml2`

Usage

```
openFile(mzml_file)
```

Arguments

`mzml_file`	the absolute file path of a valid `.mzML` file

Value

a list of two elements containing `peaks` and `header`

`parseChromNode` *Parse the XML nodeset of a SRM chromatogram*

Description

Parse the XML nodeset of a SRM chromatogram

Usage

```
parseChromNode(x, mode)
```

Arguments

`x`	a `xml2` nodeset for a `Chromatogram` block
`mode`	a character of either `SRM` or `TIC`

Value

a list of two elements

- **time**
  - `attributes`
  - `raw`
- **intensity**
  - `attributes`
  - `raw`

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