Package 'MRMConverteR'

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Type Package

Title Convert MRM-MS .mzML files to LC-MS style .mzML files

Version 0.0.99

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Description MRMConverteR takes mzML files containing multiple MRM-
MS chromatograms and converts them to LC-
MS style scan data so that they can be processed by xcms.

License GPL (>= 3)

Depends dplyr

Imports mzR (>= 2.1.2), purrr, tools

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

BugReports https://github.com/wilsontom/MRMConverteR

LazyData TRUE

Suggests testthat, covr, msdata

RoxygenNote 6.0.1

NeedsCompilation no

R topics documented:

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convert   *Convert MRM-MS files to LC-MS style files*

Description

Convert MRM-MS `.mzML` files which contain a series of time-intensity pairs (chromatograms) to a series of LC-MS scan style `m/z`-intensity pairs.

Usage

```
convert(input, outpath, return = FALSE)
```

Arguments

input	a character stirng of the absolute file path of a MRM-MS `.mzML` file
outpath	a character string of the location to save converted files to. If NULL then `return` must be TRUE
return	logical; if TRUE then the 'peaks' list is returned from the function. `Default is FALSE`.

Details

Once the data is represented as a matrix of `m/z` and intensity pairs for each scan; the data can be further processed by open source tools such as `xcms`.

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