Package: q3ML (via r-universe)

May 19, 2026

Type Package

Title Open and Parse SRM mzML Files from Thermo Triple Quadrupole Instruments

Version 0.1.0

Description Parses selective reaction monitoring (SRM) mzML chromatograms exported from Thermo triple quadrupole instruments. The package is intended as a fallback for newer ProteoWizard-generated mzML files where chromatogram data cannot be decoded through 'mzR', while preserving output structures that are easy to compare with 'mzR' headers and chromatograms.

License GPL (>= 3)

Encoding UTF-8

LazyData true

Depends magrittr

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

RoxygenNote 7.3.2

Suggests covr, testthat (>= 3.0.0), mzR

Config/testthat/edition 3

Roxygen list(markdown = TRUE)

Config/pak/sysreqs libicu-dev libxml2-dev

Repository https://wilsontom.r-universe.dev

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RemoteUrl https://github.com/wilsontom/q3ML

RemoteRef HEAD

RemoteSha 132193fbbca597ad66b0b9c1889e181c5a276f97

Contents

`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`

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