

Package: mzrust (via r-universe)

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Type Package

Title Low-Level mzML Access via Rust

Version 0.1.0

Description Experimental low-level access to mzML files from R using the Rust mzdata crate.

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

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Description

These functions provide a small handle-based API for low-level mzML access from R. `open_mzml()` validates the file and returns an external-pointer handle. `header()` returns a data frame of per-spectrum metadata, `spectrum_count()` returns the number of indexed spectra, `spectrum()` returns a named list describing a single scan together with its peaks data frame, `peaks()` returns a data frame with `mz` and `intensity` columns for a single scan, or a list of such data frames when `scan = NULL`, and `close_mzml()` marks the handle as closed. `write_mzml()` writes a new indexed mzML file containing only spectra whose retention times fall within the inclusive `rt_min` to `rt_max` window, together with recomputed TIC and base-peak summary chromatograms for that subset.

Usage

```
open_mzml(path)
```

```
header(handle)
```

```
spectrum_count(handle)
```

```
spectrum(handle, scan)
```

```
peaks(handle, scan = NULL)
```

```
close_mzml(handle)
```

```
write_mzml(handle, output_path, rt_min = -Inf, rt_max = Inf)
```

Arguments

<code>path</code>	Path to a .mzML file. Gzipped .mzML.gz files are also supported.
<code>handle</code>	An <code>mzml_handle</code> returned by <code>open_mzml()</code> .
<code>scan</code>	A 1-based scan index. If <code>NULL</code> , return all scans as a list of peak data frames.
<code>output_path</code>	Path where the filtered mzML file will be written. Output is written as indexed .mzML. If the source handle was opened from .mzML.gz, the filtered output is gzipped as well and .gz is appended when needed. The output includes recomputed TIC and base-peak summary chromatograms for the retained spectra.
<code>rt_min</code>	Inclusive lower retention-time bound, using the same units reported by <code>header()</code> .
<code>rt_max</code>	Inclusive upper retention-time bound, using the same units reported by <code>header()</code> .

Examples

```
## Not run:
con <- open_mzml("example.mzML")
hdr <- header(con)
n <- spectrum_count(con)
sp <- spectrum(con, scan = 1L)
pk <- peaks(con, scan = 1L)
all_peaks <- peaks(con)
write_mzml(con, "subset.mzML", rt_min = 5, rt_max = 10)
close_mzml(con)

## End(Not run)
```

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