Package: CentroidR (via r-universe)

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Title CentroidR

Version 0.0.0.9000

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Description CentroidR provides the infrastructure to centroid profile spectra.

License GPL (>= 3)

URL https://github.com/adafede/CentroidR, https://adafede.github.io/CentroidR

BugReports https://github.com/adafede/CentroidR/issues

Depends R (>= 4.3.0)

Imports logger (>= 0.4.0), mzR (>= 2.36.0), optparse (>= 1.7.5), Spectra (>= 1.12.0)

Remotes bioc/mzR

Suggests R.utils, testthat

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Config/pak/sysreqs make libnetcdf-dev

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

RemoteUrl https://github.com/adafede/CentroidR

RemoteRef main

RemoteSha 3456006ad861769a63378dbceec0f6c18e7695c8

Contents

`centroid_one_file` *Centroid an mzML file with configurable parameters*

Description

This function processes an mzML file to apply centroiding with detailed controls for peak picking, smoothing, and noise estimation. It allows fine-tuning of MS1 and MS2 peak detection, optimizing spectral data analysis for various experimental needs.

Usage

```
centroid_one_file(
  file,
  pattern,
  replacement,
  min_datapoints_ms1 = 2L,
  min_datapoints_ms2 = 1L,
  mz_tol_da_ms1 = 0.002,
  mz_tol_da_ms2 = 0.005,
  mz_tol_ppm_ms1 = 5,
  mz_tol_ppm_ms2 = 10,
  mz_fun = base::mean,
  int_fun = base::sum,
  mz_weighted = TRUE
)
```

Arguments

`file`	`character(1)` Path to the input mzML file. Must be a valid, accessible mzML format file.
`pattern`	`character(1)` Regular expression pattern to match in the input file path, used for modifying the output file path.
`replacement`	`character(1)` Replacement string for altering the output file path based on the `pattern`.
`min_datapoints_ms1`	`integer(1)` (default: `2L`) Minimum datapoints to be considered for MS1 data.
`min_datapoints_ms2`	`integer(1)` (default: `1L`) Minimum datapoints to be considered for MS2 data.
`mz_tol_da_ms1`	`numeric(1)` (default: `0.002`) m/z tolerance in Daltons for MS1 data.
`mz_tol_da_ms2`	`numeric(1)` (default: `0.005`) m/z tolerance in Daltons for MS2 data.

mz_tol_ppm_ms1	numeric(1) (default: 5) m/z tolerance in parts per million (ppm) for MS1.
mz_tol_ppm_ms2	numeric(1) (default: 10) m/z tolerance in parts per million (ppm) for MS2.
mz_fun	function (default: base::mean) Function to aggregate m/z values within each peak group. Ignored if mz_weighted = TRUE.
int_fun	function (default: base::sum) Function to aggregate peak intensities within each peak group.
mz_weighted	logical(1) (default: TRUE) If TRUE, uses intensity-weighted mean for m/z value aggregation.

Details

The function processes both MS1 and MS2 data with user-defined smoothing, peak-picking, and noise estimation. File path modifications are supported via pattern and replacement.

Value

logical(1) Returns TRUE if centroiding was successful, otherwise FALSE.

Author(s)

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