Package 'rtmsEcho'

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Title Extract and Analyze EchoMS Data from Sciex Wiff Files

Version 0.2.4

Description Read raw and processed data from acoustic ejection mass spectrometry (AEMS) files produced by the Sciex EchoMS instrument. Includes functions to create interactive reader objects, extract raw intensity measurements, mass spectra, and fully-processed mass-transition intensity areas. Methods for data processing and analysis are described in Rimmer et al. (2025) <doi:10.1021/acs.analchem.5c03730>. Supports both multiple reaction monitoring (MRM) and full-scan (neutral loss and precursor ion) data formats.

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Author Mary Ashley Rimmer [aut],
Nathaniel Twarog [aut, cre],
Lei Yang [aut]

Maintainer Nathaniel Twarog <nathaniel.twarog@stjude.org>

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Contents

`exampleWiff` *Example wiff reader object*

Description

An object of class `rtmsWiffReader` produced by running newWiffReader on a .wiff and .wiff.scan file. The files in question contain multiple reaction monitoring (MRM) data measuring three mass transitions, corresponding to the detection of the compounds carbamazepine, warfarin, and verapamil. The EchoMS run included measurements of 320 ejections, each three seconds apart from 320 wells of a 384-well plate.

Usage

```
exampleWiff
```

Format

A data structure of type `rtmsWiffReader`; a description of the format can be found in the description for newWiffReader

Details

Note that the wiff reader object does not contain all data from the .wiff and .wiff.scan files. It included to demonstrate some of the basic function in the package.

`getAllFullScanAreas` *Get the total area for given masses for all wells*

Description

Get the total area for given masses for all wells

Usage

```
getAllFullScanAreas(scanfile, tic, sample, ejections, peaks)
```

Arguments

`scanfile`	A file path to a Sciex raw scan file (extension .wiff.scan) containing the raw data referenced by the .wiff file from which the other parameters were extracted
`tic`	A total ion chromatogram of the format outputby `getTIC()` or `getAllTIC()`
`sample`	The particular object from the `samples` field of the `rtmsWiffReader` object, which in this case contains binary offsets into the .wiff.scan file
`ejections`	An ejection table listing the timing and boundaries of the total ion chromatogram peaks for all shots in the run, as returned by `measureEjections()`
`peaks`	A named list of peak objects of class `rtmsPeak`

Details

The table returned includes a measurement of total area for each of the mass transitions listed in `sample`. It contains one row for each measured shot each mass transition, with the following columns:

- `shotorder`: The order of the peak within the shots fired during the run
- `well`: The alphanumeric well name of the well from which the shot was fired
- `time`: The time (in seconds) after the beginning of the run at which the intensity from the shot was at its peak
- `massindex`: The index of the measured mass transition in the set of masses in the given sample
- `mass`: The name of the mass transition measured (often a compound name or id)
- `area`: The intensity area (in counts) for that particular mass transition from that ejection

Value

A data frame containing the total intensity for each `rtmsPeak` given and each ejection; see Details for column specifics.

getAllFullScanSpectra *Extract mass spectra for all wells*

Description

Extract mass spectra for all wells

Usage

```
getAllFullScanSpectra(scanfile, tic, sample, ejections)
```

Arguments

scanfile	A file path to a Sciex raw scan file (extension .wiff.scan) containing the raw data referenced by the .wiff file from which the other parameters were extracted
tic	A total ion chromatogram of the format outputby getTIC() or getAllTIC()
sample	The particular object from the samples field of the rtmsWiffReader object, which in this case contains binary offsets into the .wiff.scan file
ejections	An ejection table listing the timing and boundaries of the total ion chromatogram peaks for all shots in the run, as returned by measureEjections()

Value

A list of objects of class rtmsSpectrum containing the full extracted mass spectra for each ejection

getAllMRMAreas *Extract the peak areas for MRM mass transitions for all wells*

Description

Extract the peak areas for MRM mass transitions for all wells

Usage

```
getAllMRMAreas(scanfile, tic, sample, ejections, removeBaseline = TRUE)
```

Arguments

scanfile	A file path to a Sciex raw scan file (extension .wiff.scan) containing the raw data referenced by the .wiff file from which the other parameters were extracted
tic	A total ion chromatogram data.frame as extracted by getTIC() or getAllTIC()
sample	A "sample" object representing a run in a .wiff file, from the samples field of an rtmsWiffReader object, containing information about the mass transitions measured in that run

`ejections`	An ejection table listing the timing and boundaries of the total ion chromatogram peaks for all shots in the run, as returned by `measureEjections()`
`removeBaseline`	If TRUE, baseline intensity for each mass transition will be subtracted from the intensities in each ejection, to account for baseline intensities measured near the lower limit of quantitation

Details

The table return includes a measurement of total area for each of the mass transitions listed in `sample`. It contains one row for each measured shot each mass transition, with the following columns:

- `shotorder`: The order of the peak within the shots fired during the run
- `well`: The alphanumeric well name of the well from which the shot was fired
- `time`: The time (in seconds) after the beginning of the run at which the intensity from the shot was at its peak
- `massindex`: The index of the measured mass transition in the set of masses in the given sample
- `mass`: The name of the mass transition measured (often a compound name or id)
- `area`: The intensity area (in counts) for that particular mass transition from that ejection

Value

A data frame containing the total intensity for each mass transition and each ejection; see Details for column specifics.

`getAllTIC` *Extract all total ion chromatograms from a Wiff file*

Description

Extract all total ion chromatograms from a Wiff file

Usage

```
getAllTIC(wiff)
```

Arguments

`wiff`	A wiff reader object of class `rtmsWiffReader`

Value

A list of total ion chromatograms of the format extracted by `getTIC()`, one for each run in the given .wiff file

Examples

```
wiff <- exampleWiff

tics <- getAllTIC(wiff)
tic <- tics[[1]]
```

`getFullScanAreas` *Get the total area for given masses for a particular well*

Description

Get the total area for given masses for a particular well

Usage

```
getFullScanAreas(scanfile, tic, sample, ejections, peaks, well)
```

Arguments

`scanfile`	A file path to a Sciex raw scan file (extension .wiff.scan) containing the raw data referenced by the .wiff file from which the other parameters were extracted
`tic`	A total ion chromatogram of the format outputby `getTIC()` or `getAllTIC()`
`sample`	The particular object from the `samples` field of the `rtmsWiffReader` object, which in this case contains binary offsets into the .wiff.scan file
`ejections`	An ejection table listing the timing and boundaries of the total ion chromatogram peaks for all shots in the run, as returned by `measureEjections()`
`peaks`	A named list of peak objects of class `rtmsPeak`
`well`	The well (a string) or well index (an integer) to be measured

Details

The table return includes a measurement of total area for each of the mass transitions listed in `sample`. It contains one row for each measured shot each mass transition, with the following columns:

- `shotorder`: The order of the peak within the shots fired during the run
- `well`: The alphanumeric well name of the well from which the shot was fired
- `time`: The time (in seconds) after the beginning of the run at which the intensity from the shot was at its peak
- `massindex`: The index of the measured mass transition in the set of masses in the given sample
- `mass`: The name of the mass transition measured (often a compound name or id)
- `area`: The intensity area (in counts) for that particular mass transition from that ejection

Value

A data frame containing the total intensity for `rtmsPeak` gvien and each ejection; see Details for column specifics.

getFullScanData *Extract raw Wiff full scan data*

Description

Extract raw Wiff full scan data

Usage

```
getFullScanData(scanfile, tic, sample, removeZeros = FALSE)
```

Arguments

scanfile	A file path to a Sciex raw scan file (extension .wiff.scan) containing the raw data referenced by the .wiff file from which the other parameters were extracted
tic	A (possibly partial) total ion chromatogram of the format output by getTIC() or getAllTIC() referring to the range of timepoints to be extracted
sample	The particular object from the samples field of the rtmsWiffReader object, which in this case contains binary offsets into the .wiff.scan file
removeZeros	If FALSE (the default) all intensity measuremens for all time points and m/z values will be extractd and returned; if TRUE, only values greater than zero will be returned; this can result in a much smaller output and may be useful for calculating areas

Details

The data frame output by the function contains all the intensity data compressed into the .wiff.scan file for the given range of times; it has the following columns:

- index: The particular row of ptic the measurement corresponds to
- time: The time (in seconds) after the beginning of the run at which the measurement was taken
- mz: The mass to charge value (in m/z) which the measurement corresponds to
- intensity: The intensity (in counts per second) that was measured for the given time and m/z value

Value

A data frame containing all raw data for the given range (see Details)

getFullScanSpectrum *Extract a full mass spectrum for a given well*

Description

Extract a full mass spectrum for a given well

Usage

```
getFullScanSpectrum(scanfile, tic, sample, ejections, well)
```

Arguments

scanfile	A file path to a Sciex raw scan file (extension .wiff.scan) containing the raw data referenced by the .wiff file from which the other parameters were extracted
tic	A total ion chromatogram of the format outputby getTIC() or getAllTIC()
sample	The particular object from the samples field of the rtmsWiffReader object, which in this case contains binary offsets into the .wiff.scan file
ejections	An ejection table listing the timing and boundaries of the total ion chromatogram peaks for all shots in the run, as returned by measureEjections()
well	The well (a string) or well index (an integer) to be measured

Value

An object of class rtmsSpectrum representing the full mass spectrum for the given well

getMRMAreas *Extract the peak areas for MRM mass transitions for a given well*

Description

Extract the peak areas for MRM mass transitions for a given well

Usage

```
getMRMAreas(scanfile, tic, sample, ejections, well, removeBaseline = TRUE)
```

Arguments

scanfile	A file path to a Sciex raw scan file (extension .wiff.scan) containing the raw data referenced by the .wiff file from which the other parameters were extracted
tic	A total ion chromatogram data.frame as extracted by getTIC() or getAllTIC()
sample	A "sample" object representing a run in a .wiff file, from the samples field of an rtmsWiffReader object, containing information about the mass transitions measured in that run
ejections	An ejection table listing the timing and boundaries of the total ion chromatogram peaks for all shots in the run, as returned by measureEjections()
well	The well (a string) or well index (an integer) to be measured
removeBaseline	If TRUE, baseline intensity for each mass transition will be subtracted from the intensities in each ejection, to account for baseline intensities measured near the lower limit of quantitation

Details

The table return includes a measurement of total area for each of the mass transitions listed in sample. It contains one row for each measured shot each mass transition, with the following columns:

- shotorder: The order of the peak within the shots fired during the run
- well: The alphanumeric well name of the well from which the shot was fired
- time: The time (in seconds) after the beginning of the run at which the intensity from the shot was at its peak
- massindex: The index of the measured mass transition in the set of masses in the given sample
- mass: The name of the mass transition measured (often a compound name or id)
- area: The intensity area (in counts) for that particular mass transition from that shot's peak

Value

A data frame containing the total intensity for each mass transition and each ejection; see Details for column specifics.

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getMRMChromatograms *Extract full chromatograms for each mass transition*

Description

Extract full chromatograms for each mass transition

Usage

```
getMRMChromatograms(scanfile, tic, sample)
```

Arguments

scanfile	A file path to a Sciex raw scan file (extension .wiff.scan) containing the raw data referenced by the .wiff file from which the other parameters were extracted
tic	A total ion chromatogram data.frame as extracted by getTIC() or getAllTIC()
sample	A "sample" object representing a run in a .wiff file, from the samples field of an rtmsWiffReader object, containing information about the mass transitions measured in that run

Value

A single data frame expressing all chromatograms in a "long" format, with the following columns:

- massindex: The index of the measured mass transition in the set of masses in the given sample
- mass: The name of the mass transition measured (often a compound name or id)
- time: The time (in seconds) at which the intensity was measured
- intensity: The intensity for the given mass transition at the given time

---

getTIC *Extract a total ion chromatogram (TIC) from a Wiff file*

Description

Extract a total ion chromatogram (TIC) from a Wiff file

Usage

```
getTIC(wiff, index = 1)
```

Arguments

wiff	A wiff reader object of class rtmsWiffReader
index	The particular run within the wiff file for which the TIC should be extracted. Defaults to 1, the first (and often only) run.

Details

The total ion chromatogram data in a .wiff file contains data for every moment at which the EchoMS took a measurement. Each measurement is represented by a single row in the returned data frame, with the following four values:

- time: The time (in seconds) after the beginning of the run at which the measurement was taken
- intensity: The total ion intensity across all masses measured
- full: Either 0 (indicating data is stored as a discrete set of targeted intensities) or 1 (indicating the data is stored as a compressed full spectrum)
- offset: The binary offset within this run's data block in the associated .wiff.scan file at which this measurement's raw data can be found
- size: The size (in bytes) of this measurment's raw data in the associated .wiff.scan file.

Value

A data frame containing the TIC data (see Details)

Examples

```
wiff <- exampleWiff

tic <- getTIC(wiff)

# Plot the first 60 seconds of the total ion chromatgram using [ggplot2]
ggplot2::ggplot(tic,ggplot2::aes(x=time,y=intensity))+
ggplot2::geom_line(color="red")+
ggplot2::xlim(0,60)
```

---

getWiffShots *List of Shot Names in a given Wiff File*

Description

List of Shot Names in a given Wiff File

Usage

```
getWiffShots(wiff)
```

Arguments

`wiff`	A wiff reader object of class `rtmsWiffReader`

Details

The .wiff file includes these shot names in the order in which they were input by the user. They are generally names of wells in a plate, but the order in which they are given by the user is not necessarily the order in which the EchoMS will sample them. By default, the EchoMS will use a more "efficient" ordering, moving back and forth across the rows of the plate. So the shot names here may not correlate in order with the measurements represented by the intensities in the total ion chromatogram.

Value

A character vector containing the shot names for all shots fired in each run in a given file. Note: *not necessarily in the correct order* (see Details).

Examples

```
wiff <- exampleWiff

shots <- getWiffShots(wiff)
```

`measureEjections` *Measure total ion chromatogram peaks to estimate ejection time*

Description

Measure total ion chromatogram peaks to estimate ejection time

Usage

```
measureEjections(
  wiff,
  efficientPath = TRUE,
  center = 3,
  guess = NULL,
  index = 1,
  shots = NULL
)

## S3 method for class 'rtmsWiffReader'
measureEjections(
  wiff,
  efficientPath = TRUE,
  center = 3,
  guess = NULL,
  index = 1,
  shots = NULL
)

## Default S3 method:
measureEjections(
  wiff,
  efficientPath = TRUE,
  center = 3,
  guess = NULL,
  index = 1,
  shots = NULL
)
```

Arguments

`wiff`	Either an ojbect of class `rtmsWiffReader`, or a data frame representing a full EchoMS total ion chromatogram as extracted by `getTIC()` or `getAllTIC()`
`efficientPath`	If `TRUE`, the extraction proceeds under the assumption that shots were fired from the wells named in `shots` using the "efficient" method of the EchoMS, which proceeds left to right across odd rows (A, C, E, etc.) and right to left across even rows (B, D, F, etc.). If `FALSE`, shots are assumed to be fired from left to right across all rows

center	A guess at the timing (in seconds) between EchoMS shots. Most runs are 3 seconds apart, but the EchoMS does permit a fast mode. If a fast mode is used, 0.3 seconds should be added to fast mode timing, as the Echo requires those 0.3 to eject a droplet
guess	If included, used as the guess for the timing of the first shot. If desired this can usually be estimated visually from a plot of the total ion chromatogram intensity. Actual shot timing will still be optimized to align with TIC intensities. If NULL (the default), the function will guess at the timing of the first shot based on existing runs.
index	The particular run within the wiff file for which the TIC should be extracted. Defaults to 1, the first (and often only) run.
shots	A list of shot names as extracted by getWiffShots(); each name should begin with an alphanumeric well name (e.g. "A01", "B7", "F15") and may contain the string "Marker" to indicate the well was used as a marker.

Details

The function assumes equally timed ejections, approximately center seconds apart, can be found in the total ion chromatogram. Once the timing of these peaks is selected, the chromatogram is analyzed to locate the boundaries of these peaks, using baseline noise or local minima to draw these boundaries. The function returns a data frame with one row for each peak, with the following columns:

- shotorder: The order within the run in which the peaks appeared
- shot: The full shot name found in shots
- marker: TRUE if the shot is indicated as coming from a marker well
- well: The standard alphanumeric well name found in the shot name
- time: The time (in seconds) after the beginning of the run at which the peak is expected to reach its maximum
- minTime: The time (in seconds) after the beginning of the run at which the peak is measured to begin
- maxTime: The time (in seconds) after the beginning of the run at which the peak is measured to end
- area: The total area (in counts, as intensity is counts per second and the extend of the peak is measured in seconds) of the peak
- height: The maximum height of the peak (in counts per second)
- width: The total width of the peak (in seconds)
- halfWidth: The width of the peak at half of its maximum intensity (in seconds)

Value

A data frame of measured ejections (see Details)

Examples

```
wiff <- exampleWiff

# Works if file is run with 3 seconds between peaks and shots are fired
# from wells in the efficient "back-and-forth" path
ejections <- measureEjections(wiff)
```

`newWiffReader` *Open a Sciex EchoMS wiff File for Reading*

Description

Open a Sciex EchoMS wiff File for Reading

Usage

```
newWiffReader(wiffFile, wiffScanFile = NULL)
```

Arguments

`wiffFile`	A valid file path to the Sciex data file (extension .wiff) containing the metadata for one or more EchoMS runs
`wiffScanFile`	An optional file path the the Sciex scan file (extension .wiff.scan) containing the full raw EchoMS data

Details

The reader object produced by this function is of class `rtmsWiffReader`, and contains the information necessary to extract more detailed data from this file and the associated .wiff.scan file. It contains the following fields:

- `wiff`: The path to the .wiff file being used
- `wiffScan`: If given, the path of the associated .wiff.scan file. Some but not all functions require this file; this will be specified in their documentation.
- `cfbf`: A list of values used to parse the .wiff file's internal CFBF structure
- `samples`: The "sample" list for the .wiff file. It is important to note that these are actually different *runs* whose data have been stored in one file. Contains data on the specific masses measured in each run.

Value

An object of class `rtmsWiffReader` (see Details)

processAllFullScanAreas *Fully process a Full Scan Wiff and scan File*

Description

A convenient wrapper function to extract all full scan areas from a file without storing the intermediate reader and ejection data structures.

Usage

```
processAllFullScanAreas(wiffFile, wiffScanFile, peaks, ...)
```

Arguments

wiffFile	A valid file path to the Sciex data file (extension .wiff) containing the metadata for one or more EchoMS runs
wiffScanFile	An file path the the Sciex scan file (extension .wiff.scan) containing the full raw EchoMS data
peaks	A named list of peak objects of class rtmsPeak, often generated by rtmsPeakList()
...	Additional arguments passed to measureEjections()

Value

A list with two objects: ejections, a data frame listing all ejections for all samples in the WIFF file, with an additional wiffSample column specifying which sample each ejection was extracted from; and massAreas, a data frame of the format returned by getAllFullScanAreas(), also with an additional wiffSample column

processAllMRMAreas *Process an MRM file in total*

Description

This is a convenience function that performs an end to end analysis of an Sciex MRM run; it can be used when the intermediate data structures (total ion chromatograms, shot lists, .wiff file readers) are not required.

Usage

```
processAllMRMAreas(wiffFile, wiffScanFile, removeBaseline = TRUE, ...)
```

Arguments

`wiffFile`	A valid file path to the Sciex data file (extension .wiff) containing the metadata for one or more EchoMS runs
`wiffScanFile`	An valid file path the the Sciex scan file (extension .wiff.scan) containing the full raw EchoMS data
`removeBaseline`	If TRUE, baseline intensity for each mass transition will be subtracted from the intensities in each ejection, to account for baseline intensities measured near the lower limit of quantitation
`...`	Additional optional parameters to be passed to `measureEjections()`

Value

A list containing two data frames: `ejections`, with all extracted TIC peaks for all runs, as output by `measureEjections()`, and `massAreas`, containing the measured areas for all mass transitoins and all peaks in all runs, as output by `getMRMAreas()`. Both data frames contain an addtional `wiffSample` column indicating which run within the file the values were extracted from.

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