Package 'qqqMS'

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Type Package

Title Peak Detection for MRM-MS data

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Description Simple wrappers for post-acquistion processing of Multiple Reaction Monitoring (MRM) Mass Spectrometry (MS) data using xcms.

License GPL (>= 3)

Depends xcms, methods

Imports MSnbase

Suggests testthat, covr

Encoding UTF-8

LazyData true

RoxygenNote 6.0.1

NeedsCompilation no

R topics documented:

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extract_targets   *Extract Targets*

Description

Use a user-defined list of MRM-MR targets to create a filtered feature values matrix

Usage

```
extract_targets(features, targets)
```

Arguments

features   a list which has been produced using the [integrate_peaks](#) function

targets   a data.frame of MRM-MS targets to extract the the xcms processed object.
                targets must contain the following columns;

- **name** the generic name of the target
- **mz** the m/z value of the target (as it appears in the raw file)
- **rt** the approximate retention time of the target

Value

a data.frame of feature values for only those which corresponds to an identified target

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integrate_peaks   *Detect and integrate MRM-MS features*

Description

Use the matchedFilter algorithim xcms for feature detection in MRM-MS which have been converted to LC-MS style .mzML files.

Usage

```
integrate_peaks(files, phenoData, pol)
```

Arguments

files   a character vector of .mzML files which have been convereted from MRM-MS
                .mzML to LC-MS style .mzML files using MRMConverteR

phenoData   a data.frame. phenoData must contain the following columns;

- **fileName** file name
- **name** sample name

                Providing these two columns are present; phenoData can contain as many other
                columns as the user wishes.

pol   a charatcer string of either 1 for positive mode or -1 for negative mode. If input
                data only contains one polarity mode, then polarity can be NULL

Value

a list of two elements

- values values for the integrated peak areas of all features detected
- definitions a data.frame of feature defintions. See [XCMSnExp-class](#) for more details

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