Package 'LCMSQA'

January 20, 2025

Title Liquid Chromatography/Mass Spectrometry (LC/MS) Quality
Assessment

Version 1.0.2

Description The goal of 'LCMSQA' is to make it easy to check the quality of
liquid chromatograph/mass spectrometry (LC/MS) experiments using a
'shiny' application. This package provides interactive data
visualizations for quality control (QC) samples, including total
ion current chromatogram (TIC), base peak chromatogram (BPC), mass
spectrum, extracted ion chromatogram (XIC), and feature detection
results from internal standards or known metabolites.

License GPL (>= 3)

Encoding UTF-8

RoxygenNote 7.2.3

Depends R (>= 4.0.0)

Imports bsplus, data.table, DT, ggplot2, methods, plotly, shiny,
shinycssloaders, shinyjs, shinyWidgets

Suggests BiocManager, xcms, MSnbase, knitr, rmarkdown

VignetteBuilder knitr

NeedsCompilation no

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Repository CRAN

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LCMSQA-package	*LC/MS Quality Assessment*

Description

The 'LCMSQA' package is designed to assess the quality of liquid chromatography/mass spectrometry (LC/MS) experiment using a user-friendly web application built with the R package 'shiny'. It utilizes the R package 'xcms' workflow for data import, visualization, and quality check of LC/MS experiments.

The application consists of four main tabs:

- Total Ion Chromatogram (and Base Peak Chromatogram)
- Extracted Ion Chromatogram (XIC)
- Mass Spectrum
- Metabolic Feature Detection

Please check the vignette for the details (Run `vignette("LCMSQA", package = "LCMSQA")`).

Details

The application needs the following inputs:

- (required) mass-spectrometry data files of quality control (QC) samples in open formats: AIA/ANDI NetCDF, mzXML, mzData and mzML.
- (optional) internal standard information in a CSV format with the columns:
  - compound: the name of compound
  - adduct: adduct type (e.g., [M+H]+)
  - mode: must be either "positive" or "negative"
  - mz: a known mass-to-charge ratio (m/z) value

In the application UI, a user can tune the following parameters:

- Set m/z and retention time of interest
  - compound (or m/z) with a ppm tolerance
  - retention time in second (min, max)
- Peak picking using the centWave method (see xcms::CentWaveParam)
  - ppm: the maximal tolerated m/z deviation in consecutive scans in ppm for the initial region of interest (ROI) definition
  - peak width: the expected approximate peak width in chromatographic space
  - signal/noise cut: the signal to noise ratio cutoff
  - m/z diff: the minimum difference in m/z dimension required for peaks with overlapping retention times
  - noise: a minimum intensity required for centroids to be considered in the first analysis step

- prefilter (>= peaks, >= intensity): the prefilter step for the first analysis step (ROI detection)
- Gaussian fit: whether or not a Gaussian should be fitted to each peak
- m/z center: the function to calculate the m/z center of the chromatographic peaks
- integration: whether or not peak limits are found through descent on the Mexican Hat filtered data
- Peak grouping using the peak density method (see xcms::PeakDensityParam)
  - bandwidth: the bandwidth (standard deviation of the smoothing kernel) to be used
  - min fraction: the minimum fraction of samples in which the peaks has to be detected to define a peak group
  - bin size: the size of overlapping slices in m/z dimension

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runQA   *Start LC/MS QA application*

Description

Runs a 'shiny' application to check the quality of LC/MS experiment. The system's default web browser will be launched automatically after the app is started.

Usage

```
runQA()
```

Value

This function normally does not return; interrupt R to stop the application (usually by pressing Ctrl + C or ESC)

Examples

```
## Please check the package vignette for details on how to use the app
if (interactive()) {
  runQA()
}
```

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