Package 'MetabolomiQCsR'

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Type Package

Title QC for LC-MS data

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Description Functions for performing QC on LC-MS.

Depends R (>= 3.0)

Imports tibble, magrittr, dplyr, purrr, xcms, massageR, tidyr, scales, ggplot2, ini, stringr, RCurl, readr, utils, WGCNA

Suggests knitr, rmarkdown, faahKO, plotly, svglite, chemhelper

License GPL (>= 2)

URL None

biocViews MassSpectrometry, Metabolomics

VignetteBuilder knitr

RoxygenNote 5.0.1

Remotes stanstrup/massageR, stanstrup/chemhelper

R topics documented:

EIC_contaminants *Find EICs that behave like contaminants*

Description

This function looks in raw LC-MS data for "features"/EICs that behave like contaminants. Behaving like contaminants in this case means that a certain m/z values is present in more than `min_time` above intensity `min_int`.

Usage

```
EIC_contaminants(raw, bin_ppm = 30, interval_ppm = 30, min_time = 5,
  merge_corr = 0.9, merge_ppm = 30, min_int = 5000)
```

Arguments

`raw`	`xcmsRaw` object to profile
`bin_ppm`	Tolerance (ppm) for initial binning of m/z values
`interval_ppm`	Tolerance for creating
`min_time`	minutes
`merge_corr`	kjh
`merge_ppm`	kjhg
`min_int`	kjhg

Value

A `tibble` containing the columns:

- **mz:** m/z of the proposed contaminant
- **EIC:** EIC of the m/z.

extract_polarity *Extract polarity from xcmsRaw object.*

Description

Extracts polarity from an xcmsRaw object. The polarity found in the majority of scans is returned.

Usage

```
extract_polarity(xraw)
```

Arguments

`xraw`	The xcmsRaw object to extract polarity from.

Value

A character string giving the polarity. Can be "positive", "negative", or "unknown".

get_cont_list *Get list of known contaminants*

Description

Get list of known contaminants

Usage

```
get_cont_list(polarity = c("positive", "negative", "unknown"), type = "URL")
```

Arguments

polarity	The polarity to get contaminants for. Can be "positive", "negative" or "unknown". If "unknown" the list specified in the MetabolomiQCsR.conf is used. MetabolomiQCsR.conf can be in the working folder or the home folder. If those are not found the package default is used (unknown will used the positive mode list).
type	If using local or remote. Only "URL" implemented which downloads a list from https://github.com/stanstrup/common_mz

Value

tbl A tibble containing the columns:

- **Monoisotopic ion mass (singly charged):** m/z of the contaminant
- **Ion type:** Notation for adduct/fragment type
- **Formula for M or subunit or sequence:** Molecular formula
- **Compound ID or species:** Name of the compound
- **Possible origin and other comments:** Suggestion for the origin of the contaminant
- **References:** Reference for the contaminant

References

https://github.com/stanstrup/common_mz

get_EICs *Get EICs from xcmsRaw object*

Description

Takes an xcmsRaw object and extracts EICs. Can do multiple ranges and exclude certain masses unlike getEIC. Can be used to extract the TIC too.

Usage

```
get_EICs(xraw, range_tbl, exclude_mz = NULL, exclude_ppm = 30,
  range_tbl_cols = c("mz_lower", "mz_upper"), BPI = FALSE)
```

Arguments

xraw	xcmsRaw object to get EIC(s)/TIC from.
range_tbl	data.frame/tibble with columns for the lower and upper m/z boundaries of EIC slice(s).
exclude_mz	Masses to exclude from the EIC. Most useful to remove contaminants from TICs.
exclude_ppm	ppm tolerance of exclude_mz
range_tbl_cols	Which columns in range_tbl holds the lower and upper range. defaults to c("mz_lower","mz_upper").
BPI	Logical selecting to calculate TIC (FALSE) or BPI.

Value

tbl A tibble containing the columns:

- **scan:** scan number
- **scan_rt:** Retention time of scan
- **intensity:** The summed intensity for each scan in the given m/z interval

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plotly_clean_tt *Make replacements in plotly tooltips*

Description

Make replacements in plotly tooltips

Usage

```
plotly_clean_tt(plotly, rep)
```

Arguments

plotly	A plotly object.
rep	A named character vector. Names are the text to replace and the string is the replacement string.

Value

A plotly object.

plot_chrom *Plot chromatogram*

Description

Plot chromatogram

Usage

```
plot_chrom(tbl, RT_col = "RT", Intensity_col = "Intensity")
```

Arguments

tbl	tbl with retention time and intensity to plot
RT_col	Name of the rentention time column
Intensity_col	Name of the intensity column

Value

a ggplot object.

plot_contaminants *Bar plot of contaminants*

Description

Bar plot of contaminants

Usage

```
plot_contaminants(data, title, x_var = "comp_name", y_var = "EIC_median")
```

Arguments

data	tbl with the contamination amounts
title	Plot title
x_var	Column name that holds the compound/contaminant names
y_var	Column name that holds the compound/contaminant values

Value

a ggplot object.

`xcmsRaw_to_tbl` *Convert raw data into a tibble of xcmsRaw objects.*

Description

Convert raw data into a tibble of xcmsRaw objects.

Usage

```
xcmsRaw_to_tbl(files)
```

Arguments

`files`	character vector of file names/paths.

Value

A `tibble` containing the columns:

- **file:** Filename without path.
- **polarity:** Character string of "positive", "negative", or "unknown".
- **raw:** The xcmsRaw objects.
- **path:** The input path (files).

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