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, pool, RMySQL, DBI, lubridate, httr, purrrlyr

Suggests knitr, rmarkdown, faahKO, plotly, svglite, chemhelper, RColorBrewer, heatmaply, listviewer

License GPL (>= 2)

URL None

biocViews MassSpectrometry, Metabolomics

VignetteBuilder knitr

RoxygenNote 6.0.1

Remotes stanstrup/massageR, stanstrup/chemhelper, rstudio/pool

R topics documented:

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closest_match   *Match list of standards to peak table*

Description

This function will match a table of standard compounds and a peak table by m/z and retention time. If there is more than one possible hit the highest intensity peak will be chosen.

Usage

```
closest_match(stds, peakTable, rt_tol = 0.25, mz_ppm = 30, rt_col = "rt",
  mz_col = "mz", int_col = "into")
```

Arguments

stds	[tibble](#) of standards to match to a peak table
peakTable	[tibble](#) containing peak table supplied by [findPeaks](#) (but converted to [tibble](#)/[data.frame](#)).
rt_tol	Retention time tolerance for matching peaks. Pay attention to the unit of your tables. rt_tol should match and stds and peakTable should use same units (i.e. minutes of seconds).
mz_ppm	ppm for matching peaks.
rt_col	Character string giving the column containing the retention times. Must be same in standards and peak table.
mz_col	Character string giving the column containing the m/z values. Must be same in standards and peak table.
int_col	Character string giving the column containing the intensities in the peak table.

Value

A vector having the length equivalent to the number of rows in stds giving the indices of the hits in peakTable.

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 final EICs after merging similar bins
min_time	Minimum time (minutes) an EIC should be above min_int to be considered a contaminant.
merge_corr	Minimum correlation between EICs to be merged.
merge_ppm	Maximum difference (ppm) between EICs to be merged.
min_int	Minimum intensity that the EIC needs to be above for a a minimum of min_time.

Value

A [tibble](#) containing the columns:

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

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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".

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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 "un-
                known". If "unknown" the list specified in the MetabolomiQCs.conf is used.
                MetabolomiQCs.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

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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, min_int = 0)
```

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.
min_int	the minimum intensity mass peak to include

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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ic_boxes   *Convert raw data into a tibble of xcmsRaw objects.*

Description

Convert raw data into a tibble of xcmsRaw objects.

Usage

```
ic_boxes(token)
```

Arguments

token	A character vector containing the ICMeter token

Value

data.frame containing information about each box registered on the token account

---

ic_measurements   *Convert raw data into a tibble of xcmsRaw objects.*

Description

Convert raw data into a tibble of xcmsRaw objects.

Usage

```
ic_measurements(token, boxQR, fromDate, toDate)
```

Arguments

token	A character vector containing the ICMeter token
boxQR	A character vector containing QR code for the box you want to query
fromDate	The starting date to draw data from
toDate	The ending date to draw data to. A maximum of one month can be draw at a time.

Value

data.frame holding all the data drawn

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ic_token   *Convert raw data into a tibble of xcmsRaw objects.*

Description

Convert raw data into a tibble of xcmsRaw objects.

Usage

```
ic_token(user, pass)
```

Arguments

user	ICMeter username
pass	ICMeter password

Value

A character vector containing the ICMeter token

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parse_filenames *Parse filenames from given string*

Description

Parse filenames from given string

Usage

```
parse_filenames(filenames, filenamemask)
```

Arguments

filenames   Character string with the filenames to parse.

filenamemask   Filename mask. Variables to capture are inclosed by "%". See examples

Value

data.frame with fields parsed from the filenames

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Examples

```
testfilenames <- c("RemoveThis_METSY_sample1___17-random_AndThis.txt",
                   "RemoveThis_METSY_sample2___21-something_AndThis.txt",
                   "RemoveThis_METSY_sample3___123-blah_AndThis.txt",
                   "RemoveThis_JDRF_SameName___1-dummyA_AndThis.txt",
                   "RemoveThis_JDRF_SameName___2-dummyB_AndThis.txt",
                   "RemoveThis_JDRF_SameName___3-dummyC_AndThis.txt",
                   "RemoveThis_this_file___name-is_wrong",
                   "RemoveThis_and_this_AndThis.txt",
                   "RemoveThis_this_one___should-work",
                   "RemoveThis_how_about___this_-_one_AndThis.txt"
                  )

defaultmask   <- "RemoveThis_%study%_%name%___%rep%-%dummy%_AndThis.txt"

parse_filenames(testfilenames,defaultmask)
```

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peak_factor   *Calculate Tailing Factor and Asymmetry Factor*

Description

Calculate Tailing Factor and Asymmetry Factor

Usage

```
peak_factor(EIC, rt, factor = "TF")
```

Arguments

EIC	EIC containing the peak to calculate for. `tibble` as produced with `get_EICs`.
rt	Retention time of the center of the peak (Numeric)
factor	to calculate. Character string either "TF" (Tailing Factor) or "ASF" (Asymmetry Factor).

Value

Numeric

References

http://www.chromforum.org/viewtopic.php?t=20079

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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.

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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.

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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.

tbl2ROI   *Convert a list of peaks (rt / m/z pairs) to a Region of Interest (ROI) list for use with* findPeaks

Description

Convert a list of peaks (rt / m/z pairs) to a Region of Interest (ROI) list for use with findPeaks

Usage

```
tbl2ROI(tbl, raw, ppm, rt_tol)
```

Arguments

tbl	tibble containing the columns "rt" and "mz". rt needs to be in seconds.
raw	xcmsRaw object to create ROI for. It needs to be a specific xcmsRaw to match retention times to scan nubmers.
ppm	ppm tolerance for the generated ROI.
rt_tol	Retention time tolerance (in sec!) for the generated ROI.

Value

List containing the ROIs. Each list contains mz, mzmin, mzmax, scmin, scmax, length (set to -1, not used by centWave) and intensity (set to -1, not used by centWave) columns.

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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.
...	further arguments to xcmsRaw.

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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