

Package ‘ptairMS’

May 30, 2024

Title Pre-processing PTR-TOF-MS Data

Version 1.12.0

Date 2020-03-18

Description This package implements a suite of methods to preprocess data from PTR-TOF-MS instruments (HDF5 format) and generates the 'sample by features' table of peak intensities in addition to the sample and feature metadata (as a single ExpressionSet object for subsequent statistical analysis). This package also permit usefull tools for cohorts management as analyzing data progressively, visualization tools and quality control. The steps include calibration, expiration detection, peak detection and quantification, feature alignment, missing value imputation and feature annotation. Applications to exhaled air and cell culture in headspace are described in the vignettes and examples. This package was used for data analysis of Gassin Delyle study on adults undergoing invasive mechanical ventilation in the intensive care unit due to severe COVID-19 or non-COVID-19 acute respiratory distress syndrome (ARDS), and permit to identify four potentiel biomarquers of the infection.

License GPL-3

Encoding UTF-8

LazyData false

BugReports <https://github.com/camilleroquencourt/ptairMS/issues>

RoxygenNote 7.2.3

Imports Biobase, bit64, chron, data.table, doParallel, DT, enviPat, foreach, ggplot2, graphics, grDevices, ggpubr, gridExtra, Hmisc, methods, minpack.lm, MSnbase, parallel, plotly, rhdf5, rlang, Rcpp, shiny, shinyscreenshot, signal, scales, stats, utils

Suggests knitr, rmarkdown, BiocStyle, testthat (>= 2.1.0), ptairData, ropls

VignetteBuilder knitr

LinkingTo Rcpp

NeedsCompilation yes

biocViews Software, MassSpectrometry, Preprocessing, Metabolomics,
PeakDetection, Alignment

git_url <https://git.bioconductor.org/packages/ptairMS>

git_branch RELEASE_3_19

git_last_commit b288c6e

git_last_commit_date 2024-04-30

Repository Bioconductor 3.19

Date/Publication 2024-05-29

Author camille Roquencourt [aut, cre]

Maintainer camille Roquencourt <camille.roquencourt@hotmail.fr>

Contents

| | |
|------------------------------------|----|
| ptairMS-package | 3 |
| aggregate | 4 |
| align | 4 |
| alignSamples | 5 |
| annotateVOC | 7 |
| calibration | 9 |
| calibrationFun | 10 |
| changeTimeLimits | 11 |
| convert_to_mzML | 11 |
| createPtrSet | 12 |
| cumulative_fit_function | 14 |
| deadTimeCorr | 15 |
| defineKnots | 15 |
| detectPeak | 17 |
| determinePeakShape | 20 |
| exportSampleMetada | 20 |
| extractEIC | 21 |
| fit_averagePeak | 21 |
| fit_averagePeak_function | 22 |
| formula2mass | 23 |
| getDirectory | 23 |
| getFileNames | 24 |
| getPeakList | 25 |
| getSampleMetadata | 26 |
| importSampleMetadata | 26 |
| impute | 27 |
| imputeMat | 28 |
| initializeFit | 28 |
| LocalMaximaSG | 30 |
| makeSubGroup | 30 |
| OptimalWindowsSG | 31 |

| | |
|----------------------------------|-----------|
| PeakList | 31 |
| plot,ptrSet,ANY-method | 33 |
| plotCalib | 34 |
| plotFeatures | 35 |
| plotPeakShape | 36 |
| plotRaw | 37 |
| plotTIC | 39 |
| ptrRaw-class | 40 |
| ptrSet-class | 41 |
| readRaw | 42 |
| resetSampleMetadata | 43 |
| rmPeakList | 44 |
| RunShinnyApp | 44 |
| setSampleMetadata | 45 |
| show,ptrRaw-method | 45 |
| show,ptrSet-method | 46 |
| snipBase | 46 |
| timeLimits | 47 |
| TransmissionCurve | 49 |
| updatePtrSet | 49 |
| width | 50 |
| writeEset | 50 |
| Index | 52 |

ptairMS-package

ptairMS: Pre-processing PTR-TOF-MS Data

Description

This package implements a suite of methods to preprocess data from PTR-TOF-MS instruments (HDF5 format) and generates the 'sample by features' table of peak intensities in addition to the sample and feature metadata (as a single ExpressionSet object for subsequent statistical analysis). This package also permit usefull tools for cohorts management as analyzing data progressively, visualization tools and quality control. The steps include calibration, expiration detection, peak detection and quantification, feature alignment, missing value imputation and feature annotation. Applications to exhaled air and cell culture in headspace are described in the vignettes and examples. This package was used for data analysis of Gassin Delyle study on adults undergoing invasive mechanical ventilation in the intensive care unit due to severe COVID-19 or non-COVID-19 acute respiratory distress syndrome (ARDS), and permit to identify four potentiel biomarquers of the infection.

Author(s)

Maintainer: camille Roquencourt <camille.roquencourt@hotmail.fr>

See Also

Useful links:

- Report bugs at <https://github.com/camilleroquencourt/ptairMS/issues>

| | |
|-----------|---|
| aggregate | <i>aggregate peakgroup for align function</i> |
|-----------|---|

Description

aggregate peakgroup for align function

Usage

```
aggregate(subGroupPeak, n.exp)
```

Arguments

| | |
|--------------|---------------------------------------|
| subGroupPeak | teh group tp aggregate |
| n.exp | number of expiration done in the file |

Value

a matrix with the median of mz, mean of ppb, ppb in background, and percentage of expiration where the peak is detected @keywords internal

| | |
|-------|---|
| align | <i>Alignment with kernel gaussian density</i> |
|-------|---|

Description

Alignment with kernel gaussian density

Usage

```
align(peakTab, ppmGroup = 70, dmzGroup = 0.001)
```

Arguments

| | |
|----------|---|
| peakTab | table with comlumn : mass, quantification, and groups number to aligned |
| ppmGroup | width of sub group created beafore density estimation in ppm |
| dmzGroup | width of sub group created beafore density estimation in Da |

Value

A list containing groups formed by alignment.

`alignSamples`*Alignment between samples*

Description

AlignSamples performs alignment between samples (i.e. the matching of variables between the peak lists within the ptrSet object) by using a kernel gaussian density (Delabriere et al, 2017). This function returns an [ExpressionSet](#), which contains the matrix of peak intensities, the sample metadata (borrowed from the input ptrSet) and the variable metadata which contains the peak intensities in the background. Two filters may be applied to:

- keep only variables with a significant higher intensity in the expirations compared to the background (i.e., a p-value less than pValGreaterThres) for at least fracExp
- keep only variables which are detected in more than fracGroup percent of the samples (or group)

If you do not want to apply those filters, set fracGroup to 0 and pValGreaterThres to 1.

Usage

```
alignSamples(  
  X,  
  ppmGroup = 70,  
  fracGroup = 0.8,  
  group = NULL,  
  fracExp = 0.3,  
  pValGreaterThres = 0.001,  
  pValLessThres = 0,  
  quantiUnit = c("ppb", "ncps", "cps")[1],  
  bgCorrected = TRUE,  
  dmzGroup = 0.001  
)
```

```
## S4 method for signature 'ptrSet'  
alignSamples(  
  X,  
  ppmGroup = 70,  
  fracGroup = 0.8,  
  group = NULL,  
  fracExp = 0.3,  
  pValGreaterThres = 0.001,  
  pValLessThres = 0,  
  quantiUnit = c("ppb", "ncps", "cps")[1],  
  bgCorrected = TRUE,  
  dmzGroup = 0.001  
)
```

Arguments

| | |
|------------------|--|
| X | ptrSet already processed by the detectPeak function |
| ppmGroup | ppm maximal width for an mz group |
| fracGroup | only variables present in fracGroup percent of at least one group will be kept (if 0 the filter is not applied) |
| group | character: sampleMetadata data column name. If NULL, variables not present in fracGroup percent of samples will be deleted. Else, variables not present in fracGroup percent in in at least one group group will be removed. |
| fracExp | fraction of samples which must have their p-value less than pValGreaterThres and pValLessThres |
| pValGreaterThres | threshold of the p-value for the unilateral testing that quantification (in cps) of expiration points are greater than the intensities in the background. |
| pValLessThres | threshold of the p-value for the unilateral testing that quantification (in cps) of expiration points are less than the intensities of the background. |
| quantiUnit | ppb, ncps or cps |
| bgCorrected | logical: should the peak table contain the background corrected values? |
| dmzGroup | minimum mz width to be used for grouping the features (required for low masses) |

Value

an [ExpressionSet](#) (Biobase object)

References

Delabriere et al., 2017

Examples

```
library(ptairData)
dirRaw <- system.file("extdata/exhaledAir", package = "ptairData")
exhaledPtrset <- createPtrSet(dir=dirRaw,
setName="exhaledPtrset", mzCalibRef = c(21.022, 60.0525),
fracMaxTIC = 0.7, saveDir = NULL )
exhaledPtrset<-detectPeak(exhaledPtrset,mzNominal=c(21,60,79))
eset <- alignSamples(exhaledPtrset,pValGreaterThres=0.05)
Biobase::exprs(eset)
Biobase::fData(eset)
Biobase::pData(eset)
```

| | |
|-------------|--|
| annotateVOC | <i>Putative annotation of VOC m/z by using the reference compilation from the literature</i> |
|-------------|--|

Description

Putatively annotate VOC m/z by using the reference compilation from the literature, and propose an isotope detection.

Usage

```
annotateVOC(  
  x,  
  ionMassColname = "ion_mass",  
  ppm = 20,  
  prefix = "vocDB_",  
  fields = c("ion_mass", "ion_formula", "formula", "mass_monoiso", "name_iupac",  
            "pubchem_cid", "inchi", "inchikey", "ref_year", "ref_pmid", "disease_name",  
            "disease_meshid")[c(1, 2, 5)]  
)  
  
## S4 method for signature 'ExpressionSet'  
annotateVOC(  
  x,  
  ionMassColname = "ion_mass",  
  ppm = 50,  
  prefix = "vocDB_",  
  fields = c("ion_mass", "ion_formula", "formula", "mass_monoiso", "name_iupac",  
            "pubchem_cid", "inchi", "inchikey", "ref_year", "ref_pmid", "disease_name",  
            "disease_meshid")[c(1, 2, 5)]  
)  
  
## S4 method for signature 'data.frame'  
annotateVOC(  
  x,  
  ionMassColname = "ion_mass",  
  ppm = 50,  
  prefix = "vocDB_",  
  fields = c("ion_mass", "ion_formula", "formula", "mass_monoiso", "name_iupac",  
            "pubchem_cid", "inchi", "inchikey", "ref_year", "ref_pmid", "disease_name",  
            "disease_meshid")[c(1, 2, 5)]  
)  
  
## S4 method for signature 'numeric'  
annotateVOC(  
  x,  
  ionMassColname = "",
```

```

ppm = 50,
prefix = "vocDB_",
fields = c("ion_mass", "ion_formula", "formula", "mass_monoiso", "name_iupac",
  "pubchem_cid", "inchi", "inchikey", "ref_year", "ref_pmid", "disease_name",
  "disease_meshid")[c(1, 2, 5)]
)

```

Arguments

| | |
|----------------|--|
| x | Expression set object (resp. data.frame) (resp. numeric vector) containing the PTR-MS processed data (resp. containing a column with the ion mass values) (resp. containing the ion mass values) |
| ionMassColname | Character: column name from the fData (resp. from the data.frame) containing the ion mass values; [default: 'ion_mass']; this argument is not used when x is a numeric vector |
| ppm | Numeric: tolerance |
| prefix | Character: prefix for the new 'annotation' columns [default: 'vocDB_'] |
| fields | Character vector: fields of the 'vocDB' database to be queried among: 'ion_mass' [default], 'ion_formula' [default], 'formula', 'mass_monoiso', 'name_iupac' [default], 'pubchem_cid', 'inchi', 'inchikey', 'ref_year', 'ref_pmid', 'disease_name', 'disease_meshid' |

Value

Returns the data.frame with additional columns containing the vocDB informations for the matched ion_mass values as well as the detected isotopes

Examples

```

dirRaw <- system.file("extdata/exhaledAir", package = "ptairData")
exhaledPtrset <- createPtrSet(dir=dirRaw,
setName="exhaledPtrset", mzCalibRef = c(21.022, 60.0525),
fracMaxTIC = 0.7, saveDir = NULL )
exhaledPtrset<-detectPeak(exhaledPtrset,mz=c(21,59,77))
exhaled.eset <-alignSamples(exhaledPtrset ,pValGreaterThres=0.05)
# Expression Set
exhaled.eset <- annotateVOC(exhaled.eset)
head(Biobase::fData(exhaled.eset))
# Data frame
exhaled_fdata.df <- Biobase::fData(exhaled.eset)
exhaled_fdata.df <- annotateVOC(exhaled_fdata.df)
head(exhaled_fdata.df)
# Numeric
ionMass.vn <- as.numeric(Biobase::featureNames(exhaled.eset))
annotated_ions.df <- annotateVOC(ionMass.vn)
head(annotated_ions.df)

```

`calibration`*Calibrates the mass axis with references masses*

Description

To convert Time Of Flight (TOF) axis to mass axis, we use the formula: $mz = ((tof-b)/a)^2$ (Muller et al. 2013) To estimate those parameters, references peaks with accurate know masses and without overlapping peak are needed. The best is that the references masses covers a maximum of the mass range.

Usage

```
calibration(  
  x,  
  mzCalibRef = c(21.022, 29.013424, 41.03858, 60.0525, 203.943, 330.8495),  
  calibrationPeriod = 60,  
  tol = 70,  
  ...  
)  
  
## S4 method for signature 'ptrRaw'  
calibration(  
  x,  
  mzCalibRef = c(21.022, 29.013424, 41.03858, 59.049141, 75.04406, 203.943, 330.8495),  
  calibrationPeriod = 60,  
  tol = 70,  
  ...  
)  
  
## S4 method for signature 'ptrSet'  
calibration(  
  x,  
  mzCalibRef = c(21.022, 29.013424, 41.03858, 75.04406, 203.943, 330.8495),  
  calibrationPeriod = 60,  
  tol = 70,  
  fileNames = getParameters(x)$listFile  
)
```

Arguments

| | |
|--------------------------------|--|
| <code>x</code> | a ptrRaw-class or ptrSet-class object |
| <code>mzCalibRef</code> | Vector of accurate mass values of intensive peaks and 'unique' in a nominal mass interval (without overlapping) |
| <code>calibrationPeriod</code> | in second, coefficient calibration are estimated for each sum spectrum of <code>calibrationPeriod</code> seconds |

```

tol          the maximum error tolerated in ppm. If more than tol warnings.
...          " "
fileNames    file to recalibrate

```

Value

the same ptrRaw or ptrSet as in input, with the following modified element:

- mz: the new mz axis calibrated
- rawM: same raw matrix with the new mz axis in rownames
- calibMassRef: reference masses used for the calibration
- calibMzToTof and calibTofToMz: function to convert TOF to mz
- calibError: the calibration error to the reference masses in ppm
- calibrationIndex: index time of each calibration period

Examples

```

### ptrRaw object

library(ptairData)
filePath <- system.file('extdata/exhaledAir/ind1', 'ind1-1.h5',
package = 'ptairData')
raw <- readRaw(filePath, calib = FALSE)
rawCalibrated <- calibration(raw)

```

| | |
|----------------|-----------------------------|
| calibrationFun | <i>calibration function</i> |
|----------------|-----------------------------|

Description

Performs calibration on sp with mzCalibRef reference masses and mzToTofFunc as previous calibration function

Usage

```
calibrationFun(sp, mz, mzCalibRef, calibCoef, peakShape, tol)
```

Arguments

| | |
|------------|--|
| sp | spectrum |
| mz | mass axis |
| mzCalibRef | masses of know reference peaks |
| calibCoef | coefficient of the previous calibration |
| peakShape | a list with reference axis and a reference peak shape centered in zero |
| tol | maximum error tolerated in ppm |

Value

list

| | |
|------------------|--|
| changeTimeLimits | <i>Shinny application to modify and view expiration limits This function run a shiny app, where you can check the automatic expiration detection, knots location, and modify it.</i> |
|------------------|--|

Description

Shinny application to modify and view expiration limits

This function run a shiny app, where you can check the automatic expiration detection, knots location, and modify it.

Usage

```
changeTimeLimits(ptrSet)
```

Arguments

ptrSet a ptrSet object

Value

the ptrSet object modified

Examples

```
library(ptairData)
directory <- system.file("extdata/exhaledAir", package = "ptairData")
ptrSet <- createPtrSet(directory, setName="ptrSet", mzCalibRef=c(21.022, 59.049),
  fracMaxTIC=0.8)
## Not run: ptrSet <- changeTimeLimits(ptrSet)
```

| | |
|-----------------|----------------------------------|
| convert_to_mzML | <i>Convert a h5 file to mzML</i> |
|-----------------|----------------------------------|

Description

convert_to_mzML create a mzML file from a h5 file in the same directory with the writeMLData of the MSnbase package

Usage

```
convert_to_mzML(file)
```

Arguments

file A .h5 file path

Value

create a mzML file in the same directory of the h5 input file

Examples

```
library(ptairData)
filePathRaw <- system.file('extdata/exhaledAir/ind1', 'ind1-1.h5',
package = 'ptairData')
# write a mzml file in the same directory
convert_to_mzML(filePathRaw)
file_mzML <- gsub(".h5", ".mzML", filePathRaw)
file.remove(file_mzML)
```

| | |
|--------------|---|
| createPtrSet | <i>Creates a ptrSet object form a directory</i> |
|--------------|---|

Description

This function creates a [ptrSet-class](#) S4 object. It opens each file and:

- performs an external calibration by using the `mzCalibRef` reference masses on the sum spectra every `calibrationPeriod` second
- quantifies the primary ion (H3O+ isotope by default) on the average total ion spectrum.
- calculates expiration on the `mzBreathTracer` trace. The part of the trace where the intensity is higher than `fracMaxTIC * max(trace)` is considered as expiration. If `fracMaxTIC` is different to zero, this step is skipped
- defines the set of knots for the peak analysis (see [detectPeak](#))
- provides a default `sampleMetadata` based on the tree structure of the directory and the acquisition date (a `data.frame` with file names as row names)
- If `saveDir` is not `NULL`, the returned object will be saved as a `.Rdata` in `saveDir` with the `setName` as name

Usage

```
createPtrSet(
  dir,
  setName,
  mzCalibRef = c(21.022, 29.013424, 41.03858, 60.0525, 203.943, 330.8495),
  calibrationPeriod = 60,
  fracMaxTIC = 0.8,
  mzBreathTracer = NULL,
  knotsPeriod = 3,
```

```

    mzPrimaryIon = 21.022,
    saveDir = NULL
)

```

Arguments

| | |
|-------------------|--|
| dir | character. a directory path which contains several h5 files, possibly organized in subfolder |
| setName | character. name of the ptrSet object. If 'saveDir' is not null, the object will be saved with this name. |
| mzCalibRef | vector of the reference mass values; those masses should be accurate, and the corresponding peaks should be of high intensity and 'unique' in a nominal mass interval (without overlapping peaks) to performs calibration. See ?calibration. |
| calibrationPeriod | in second, coefficient calibration are estimated for each sum spectrum of calibrationPeriod seconds |
| fracMaxTIC | Fraction (between 0 and 1) of the maximum of the Total Ion Current (TIC) amplitude after baseline removal. Only the part of the spectrum where the TIC intensity is higher than 'fracMaxTIC * max(TIC)' will be analyzed. If you want to analyze the entire spectrum, set this parameter to 0. |
| mzBreathTracer | integer: nominal mass of the Extracted Ion Current (EIC) used to compute the expiration time limits. If NULL, the limits will be computed on the Total Ion Current (TIC). |
| knotsPeriod | period in second (time scale) between two knots for the two dimensional modeling |
| mzPrimaryIon | Exact mass of the primary ion isotope |
| saveDir | Directory where the ptrSet object will be saved as .RData. If NULL, nothing will be saved. |

Value

a ptrSet object with slots :

- Parameter: list containing the parameters used for createPrtSet, detectPeak and alignTimePeriods functions.
- sampleMetadata: data frame containing information about the data, with file names in row names
- mzCalibRef: list containing for each file the masses used for the calibration (see ?ptairMS::calibration for more details)
- signalCalibRef: mz and intensity +/- 0.4Da around the calibration masses
- errorCalibPpm: list containing for each file the accuracy error in ppm at each calibration masses
- coefCalib: list containing the calibration coefficients 'a' and 'b' which enable to convert tof to mz for each file (see [calibration](#) function for more details).
- resolution: estimated resolution $m/\Delta m$ for each calibration masses within each file

- TIC: The Total Ion Current for each file
- timeLimit: list containing, for each file, a list of two element: the matrix of time limit for each file (if fracMaxTIC is different to zero), and the background index. See [timeLimits](#) for more details
- peakList: list containing for each file an expression set [eSet](#), with m/z peak center, quantification for background and exhaled air in cps, ppb and ncps, and quantity for each time points. See [getPeakList](#) for more details.

Examples

```
library(ptairData)
directory <- system.file('extdata/mycobacteria', package = 'ptairData')
ptrSet<-createPtrSet(dir=directory, setName='ptrSet'
, mzCalibRef=c(21.022, 59.049),
fracMaxTIC=0.9, saveDir= NULL)
```

cumulative_fit_function

Create cumulative function fit

Description

Create cumulative function fit

Usage

```
cumulative_fit_function(fit_function_str, par_var_str, par_fix_str, n.peak)
```

Arguments

| | |
|------------------|--|
| fit_function_str | fit function who will be use in character |
| par_var_str | parameters of fit function who change with the peak in a vector of character |
| par_fix_str | parameters of fit function independent of the peak in a vector of character |
| n.peak | number of peak |

Value

a list:
 init.names: names of paramters for the initialization
 func.eval: function who will be fitted

| | |
|--------------|---|
| deadTimeCorr | <i>Dead time correction on raw data</i> |
|--------------|---|

Description

Dead time correction on raw data

Usage

```
deadTimeCorr(raw, ve, vne, r, threshold = 0.1)
```

Arguments

| | |
|-----------|--|
| raw | ptrRaw object |
| ve | extending dead time |
| vne | non extending dead time |
| r | number of extraction |
| threshold | only bin of intensity more then threshold*r which be corrected |

Value

a ptrRaw object with the raw matrix corrected

| | |
|-------------|----------------------------------|
| defineKnots | <i>Define the knots location</i> |
|-------------|----------------------------------|

Description

defineKnots function determine the knots location for a ptrSet or ptrRaw object. There is three possibilities :

- method = expiration in the expiration periods, a knots is placed every knotsPeriod seconds, and 1 knots in the middle of two expiration, one at begin and at the end
- method= uniforme, the knots are placed uniformly every knotsPeriod time points
- give in knotsList a list of knot, with all base name file in name of the list element. All file must be informed. The knots location must be contained in the time axis

Usage

```

defineKnots(
  object,
  knotsPeriod = 3,
  method = c("expiration", "uniform", "manual")[1],
  knotsList = NULL,
  ...
)

## S4 method for signature 'ptrRaw'
defineKnots(
  object,
  knotsPeriod = 3,
  method = c("expiration", "uniform")[1],
  knotsList = NULL,
  timeLimit = list(NULL)
)

## S4 method for signature 'ptrSet'
defineKnots(
  object,
  knotsPeriod = 3,
  method = c("expiration", "uniform")[1],
  knotsList = NULL
)

```

Arguments

| | |
|-------------|---|
| object | ptrSet object |
| knotsPeriod | the period in second (times scale) between two knots for the two dimensional modelization |
| method | expiration or uniform |
| knotsList | a list of knot location for each files, with all base name file in name of the list element |
| ... | not used |
| timeLimit | index time of the expiration limits and background |

Value

numeric vector of knots
a list with numeric vector of knots for each file

Examples

```

library(ptairData)
dirRaw <- system.file("extdata/exhaledAir", package = "ptairData")
exhaledPtrset <- createPtrSet(dir=dirRaw, setName="exhaledPtrset",

```



```

mzCalibRef = c(21.022, 60.0525), fracMaxTIC = 0.7, saveDir = NULL )

#### placed knots every 2 times points
exhaledPtrset <- defineKnots(exhaledPtrset ,knotsPeriod=2,method='uniform')

#### placed knots every 3 times points in the expiration (default)
exhaledPtrset <- defineKnots(exhaledPtrset ,knotsPeriod=3,method='expiration')

```

detectPeak

Detection and quantification of peaks for a ptrSet object.

Description

The detectPeak function detects peaks on the average total spectrum around nominal masses, for all files present in ptrSet which have not already been processed. The temporal evolution of each peak is then evaluated by using a two-dimensional penalized spline regression. Finally, the expiration points (if defined in the ptrSet) are averaged, and a t-test is performed between expiration and ambient air. The peakList can be accessed with the [getPeakList](#) function, which returns the information about the detected peaks in each file as a list of ExpressionSet objects. The peak detection steps within each file are as follows:

for each nominal mass:

- correction of the calibration drift
- peak detection on the average spectrum
- estimation of temporal evolution
- t-test between expiration and ambient air

Usage

```

detectPeak(
  x,
  ppm = 130,
  minIntensity = 10,
  minIntensityRate = 0.01,
  mzNominal = NULL,
  resolutionRange = NULL,
  fctFit = NULL,
  smoothPenalty = NULL,
  parallelize = FALSE,
  nbCores = 2,
  saving = TRUE,
  saveDir = getParameters(x)$saveDir,
  ...
)

## S4 method for signature 'ptrRaw'
detectPeak(

```

```

x,
ppm = 130,
minIntensity = 10,
minIntensityRate = 0.01,
mzNominal = NULL,
resolutionRange = NULL,
fctFit = NULL,
smoothPenalty = NULL,
timelimit,
knots = NULL,
mzPrimaryIon = 21.022,
...
)

## S4 method for signature 'ptrSet'
detectPeak(
  x,
  ppm = 130,
  minIntensity = 10,
  minIntensityRate = 0.01,
  mzNominal = NULL,
  resolutionRange = NULL,
  fctFit = NULL,
  smoothPenalty = 0,
  parallelize = FALSE,
  nbCores = 2,
  saving = TRUE,
  saveDir = getParameters(x)$saveDir,
  ...
)

```

Arguments

| | |
|------------------|---|
| x | a <code>ptrSet</code> object |
| ppm | minimum distance in ppm between two peaks |
| minIntensity | minimum intensity for peak detection. The final threshold for peak detection will be: $\max(\text{minIntensity}, \text{threshold noise})$. The threshold noise corresponds to $\max(\max(\text{noise around the nominal mass}), \text{minIntensityRate} * \max(\text{intensity within the nominal mass}))$ |
| minIntensityRate | Fraction of the maximum intensity to be used for noise thresholding |
| mzNominal | nominal masses at which peaks will be detected; if NULL, all nominal masses of the mass axis |
| resolutionRange | vector with the minimum, average, and maximum resolution of the PTR instrument. If NULL, the values are estimated by using the calibration peaks. |
| fctFit | function for the peak quantification: should be <code>sech2</code> or <code>averagePeak</code> . If NULL, the best function is selected by using the calibration peaks |

| | |
|---------------|--|
| smoothPenalty | second order penalty coefficient of the p-spline used for two-dimensional regression. If NULL, the coefficient is estimated by generalized cross validation (GCV) criteria |
| parallelize | Boolean. If TRUE, loops over files are parallelized |
| nbCores | number of cluster to use for parallel computation. |
| saving | boolean. If TRUE, the object will be saved in saveDir with the setName parameter of the createPtrSet function |
| saveDir | The directory where the ptrSet object will be saved as .RData. If NULL, nothing will be saved |
| ... | may be used to pass parameters to the processFileTemporal function |
| timeLimit | index time of the expiration limits and background. Should be provided by timeLimits function |
| knots | numeric vector corresponding to the knot values, which used for the two dimensional regression for each file. Should be provided by defineKnots function |
| mzPrimaryIon | the exact mass of the primary ion isotope |

Value

an S4 ptrSet object, that contains the input ptrSet completed with the peakLists.

References

Muller et al 2014, Holzinger et al 2015, Marx and Eilers 1992

Examples

```
## For ptrRaw object
library(ptairData)
filePath <- system.file('extdata/exhaledAir/ind1', 'ind1-1.h5',
package = 'ptairData')
raw <- readRaw(filePath,mzCalibRef=c(21.022,59.049),calib=TRUE)
timeLimit<-timeLimits(raw,fracMaxTIC=0.7)
knots<-defineKnots(object = raw,timeLimit=timeLimit)
raw <- detectPeak(raw, timeLimit=timeLimit, mzNominal = c(21,59),
smoothPenalty=0,knots=knots,resolutionRange=c(2000,5000,8000))

## For a ptrSet object
library(ptairData)
directory <- system.file("extdata/exhaledAir", package = "ptairData")
exhaledPtrset<-createPtrSet(dir=directory,setName="exhaledPtrset",
mzCalibRef=c(21.022,59.049),
fracMaxTIC=0.9,saveDir= NULL)
exhaledPtrset <- detectPeak(exhaledPtrset)
peakListEset<-getPeakList(exhaledPtrset)
Biobase::fData(peakListEset[[1]])
Biobase::exprs(peakListEset[[1]])
```

determinePeakShape *Determine peak shape from raw data in tof*

Description

This function use the method describe by average and al 2013, for determine a peak shape from the raw data :

$\$peak_i(\Delta_i, A_i, t_i) = \text{interpolation}(x = \text{tof.ref} * \Delta_i + t_i, y = A_i * \text{peak.ref}, xout = \text{TOF}_i)$ where peak.ref and tof.ref are peaks reference use for mass calibration.

Usage

```
determinePeakShape(raw, plotShape = FALSE)
```

Arguments

raw a ptrRaw-class object
 plotShape if true plot each reference peak and the average peak (the peak shape)

Value

A list of two vectors which are the reference peak normalized tof and intensity.

exportSampleMetada *export sampleMetadata*

Description

export sampleMetadata

Usage

```
exportSampleMetada(set, saveFile)
```

Arguments

set a ptrSet object
 saveFile a file path in tsv extension where the data.frame will be exported

Value

nothing

Examples

```
dirRaw <- system.file("extdata/exhaledAir", package = "ptairData")
exhaledPtrset <- createPtrSet(dir=dirRaw, setName="exhaledPtrset",
mzCalibRef = c(21.022, 60.0525), fracMaxTIC = 0.7, saveDir = NULL )
saveFile<-file.path(getwd(), 'sampleMetadata.tsv')
#exportSampleMetada(exhaledPtrset ,saveFile)
```

| | |
|------------|--|
| extractEIC | <i>extract all raw EIC from a pre-definied peak List</i> |
|------------|--|

Description

extract all raw EIC from a pre-definied peak List

Usage

```
extractEIC(raw, peak, peakQuantil = 0.01, fctFit = "sech2")
```

Arguments

| | |
|-------------|---|
| raw | ptrRaw object |
| peak | a data.frame with a column named 'Mz'. The Mz of the VOC detected |
| peakQuantil | the quantile of the peak shape to determine the borne of the EIC |
| fctFit | function used to fit peak |

Value

list containing all EIC and the mz borne for all peak

| | |
|-----------------|---------------------------------------|
| fit_averagePeak | <i>Fit peak with average function</i> |
|-----------------|---------------------------------------|

Description

Fit peak with average function

Usage

```
fit_averagePeak(initTof, l.shape, sp, bin, lower.cons, upper.cons)
```

Arguments

| | |
|------------|-------------------------------|
| initTof | list of initialisation in tof |
| l.shape | peak shape average |
| sp | spectrum |
| bin | tof axis |
| lower.cons | lower constrain for fit |
| upper.cons | upper constrain for fit |

Value

list with fit information

fit_averagePeak_function
fit function average

Description

fit function average

Usage

fit_averagePeak_function(t, delta, h, intervRef, peakShape, bin)

Arguments

| | |
|-----------|-------------------------------------|
| t | tof center of peak |
| delta | FWHM of peak |
| h | peak height |
| intervRef | reference interval for peak shape |
| peakShape | peak shape estimated on intervalRef |
| bin | bin interval of peak will be fitted |

Value

peak function made on an average of reference peaks normalized

| | |
|--------------|----------------------------|
| formula2mass | <i>Compute exact mass.</i> |
|--------------|----------------------------|

Description

Compute exact mass from an elemental formula

Usage

```
formula2mass(formula.vc, protonate.l = TRUE)
```

Arguments

| | |
|-------------|--|
| formula.vc | Vector of molecular formulas. |
| protonate.l | Should a proton be added to the formula? |

Value

Vector of the corresponding (protonated) masses.

Examples

```
formula2mass("CO2")
```

| | |
|--------------|--|
| getDirectory | <i>get the files directory of a ptrSet</i> |
|--------------|--|

Description

get the files directory of a ptrSet

Usage

```
getDirectory(ptrSet)
```

Arguments

| | |
|--------|---------------|
| ptrSet | ptrSet object |
|--------|---------------|

Value

the directory in absolute path as character

Examples

```
library(ptairData)
dirRaw <- system.file("extdata/exhaledAir", package = "ptairData")
exhaledPtrset <- createPtrSet(dir=dirRaw, setName="exhaledPtrset",
mzCalibRef = c(21.022, 60.0525), fracMaxTIC = 0.7, saveDir = NULL )
getDirectory(exhaledPtrset )
```

| | |
|--------------|---|
| getFileNames | <i>get the file names containing in the directory of a ptrSet or ptrRaw</i> |
|--------------|---|

Description

get the file names containing in the directory of a ptrSet or ptrRaw

get the file names containing in the directory of a ptrSet

Usage

```
getFileNames(object, fullNames = FALSE)
```

```
## S4 method for signature 'ptrSet'
getFileNames(object, fullNames = FALSE)
```

```
## S4 method for signature 'ptrRaw'
getFileNames(object, fullNames = FALSE)
```

Arguments

object ptrSet object

fullNames logical: if TRUE, it return the the directory path is prepended to the file names.

Value

a vector of character that contains all file names

Examples

```
library(ptairData)
dirRaw <- system.file("extdata/exhaledAir", package = "ptairData")
exhaledPtrset <- createPtrSet(dir=dirRaw, setName="exhaledPtrset",
mzCalibRef = c(21.022, 60.0525), fracMaxTIC = 0.7, saveDir = NULL )
getFileNames(exhaledPtrset )
```

| | |
|-------------|---|
| getPeakList | <i>get the peak list of a ptrSet object</i> |
|-------------|---|

Description

get the peak list of a ptrSet object

Usage

```
getPeakList(set)
```

Arguments

| | |
|-----|---------------|
| set | ptrSet object |
|-----|---------------|

Value

a list of expressionSet, where:

- assay Data contains the matrix with m/z peak center in row names, and the quantification in cps at each time point
- feature Data the matrix with m/z peak center in row names, and the following columns:
 - quanti_unit: the mean of the quantification over the expiration/headspace time limits defined
 - background_unit: the mean of the quantification over the background time limits defined
 - diffAbs_unit: the mean of the quantification over the expiration/headspace time limits defined after subtracting the baseline estimated from the background points defined
 - pValLess/ pValGreater: the p-value of the unilateral t-test, who test that quantification (in cps) of expiration points are less/greater than the intensity of the background.
 - lower/upper: integration boundaries
 - parameter peak: estimated peak parameter

Examples

```
library(ptairData)
dirRaw <- system.file("extdata/exhaledAir", package = "ptairData")
exhaledPtrset <- createPtrSet(dir=dirRaw, setName="exhaledPtrset",
mzCalibRef = c(21.022, 60.0525), fracMaxTIC = 0.7, saveDir = NULL )
exhaledPtrset<-detectPeak(exhaledPtrset,mz=c(21,59))
peakList<- getPeakList(exhaledPtrset )
X<-Biobase::exprs(peakList[[1]])
Y<- Biobase::fData(peakList[[1]])
head(Y)
```

getSampleMetadata *get sampleMetadata of a ptrSet*

Description

get sampleMetadata of a ptrSet

Usage

```
getSampleMetadata(set)
```

Arguments

set a ptrSet object

Value

a data.frame

Examples

```
dirRaw <- system.file("extdata/exhaledAir", package = "ptairData")
exhaledPtrset <- createPtrSet(dir=dirRaw, setName="exhaledPtrset",
mzCalibRef = c(21.022, 60.0525), fracMaxTIC = 0.7, saveDir = NULL)
SMD<-getSampleMetadata(exhaledPtrset)
```

importSampleMetadata *import a sampleMetadata from a tsv file to a ptrSet object*

Description

import a sampleMetadata from a tsv file to a ptrSet object

Usage

```
importSampleMetadata(set, file)
```

Arguments

set a ptrSet object
file a tsv file contains the sample metadata to import, with all file names in row name
(the first column on the excel).

Value

a ptrSet with the new sample Metadata

Examples

```
library(ptairData)
dirRaw <- system.file("extdata/exhaledAir", package = "ptairData")
exhaledPtrset <- createPtrSet(dir=dirRaw, setName="exhaledPtrset",
mzCalibRef = c(21.022, 60.0525), fracMaxTIC = 0.7, saveDir = NULL )
saveFile<-file.path(getwd(), 'sampleMetadata.tsv')
#exportSampleMetada(exhaledPtrset ,saveFile)
#exhaledPtrset<-importSampleMetadata(exhaledPtrset ,saveFile)
```

impute

Imputes the missing values

Description

Imputes missing values by returning back to the raw data and fitting the peak shape function on the noise (or on the residuals signals if peaks have already been detected).

Usage

```
impute(eSet, ptrSet, parallelize = FALSE, nbCores = 2)
```

Arguments

| | |
|-------------|--|
| eSet | ExpressionSet returned by the alignSamples function |
| ptrSet | ptrSet-class object processed by the detectPeak function |
| parallelize | boolean. If TRUE, the loop over all files will be parallelized |
| nbCores | number of clusters to use for parallel computation. |

Value

the same ExpressionSet as in input, with the imputed missing values in the assayData slot

Examples

```
library(ptairData)
dirRaw <- system.file("extdata/exhaledAir", package = "ptairData")
exhaledPtrset <- createPtrSet(dir=dirRaw,
setName="exhaledPtrset", mzCalibRef = c(21.022, 60.0525),
fracMaxTIC = 0.7, saveDir = NULL )
exhaledPtrset<-detectPeak(exhaledPtrset,mz=c(21,52))
eSet <- alignSamples(exhaledPtrset,pValGreaterThres=0.05,fracGroup=0)
Biobase::exprs(eSet)
eSet <- impute(eSet,exhaledPtrset)
Biobase::exprs(eSet)
```

| | |
|-----------|--|
| imputeMat | <i>Impute missing values on an matrix set from an ptrSet</i> |
|-----------|--|

Description

Imputing missing values by returning back to the raw data and fitting the peak shape function on the noise / residuals

Usage

```
imputeMat(X, ptrSet, quantiUnit)
```

Arguments

| | |
|------------|---|
| X | the peak table matrix with missing values |
| ptrSet | processed by detectPeak function |
| quantiUnit | the unit of the quantities in the matrix X (ppb, cps or ncps) |

Value

the same matrix as in input, with missing values imputing

Examples

```
library(ptairData)
dirRaw <- system.file("extdata/exhaledAir", package = "ptairData")
exhaledPtrset <- createPtrSet(dir=dirRaw,
setName="exhaledPtrset", mzCalibRef = c(21.022, 60.0525),
fracMaxTIC = 0.7, saveDir = NULL )
exhaledPtrset<-detectPeak(exhaledPtrset,mz=c(21,52))
eSet <- alignSamples(exhaledPtrset,pValGreaterThres=0.05,fracGroup=0)
X <-Biobase::exprs(eSet)
X <- imputeMat(X,exhaledPtrset,quantiUnit='ppb')
plotFeatures(exhaledPtrset,mz = 52.047,typePlot = "ggplot",colorBy = "subfolder")
```

| | |
|---------------|--|
| initializeFit | <i>initialization for apply fit function in the spectrum</i> |
|---------------|--|

Description

initialization for apply fit function in the spectrum

Usage

```
initializeFit(  
  i,  
  sp.i.fit,  
  sp.i,  
  mz.i,  
  calibCoef,  
  resmean,  
  minpeakheight,  
  noiseacf,  
  ppmPeakMinSep,  
  daSeparation,  
  d,  
  plotAll,  
  c  
)
```

Arguments

| | |
|---------------|--|
| i | the nominal mass |
| sp.i.fit | the vector who will be fettet (spectrum pf residual) |
| sp.i | the spectrum around a nominal mass |
| mz.i | the mass vector around a nominal mass |
| calibCoef | calibration coeficient |
| resmean | resolution $m/\Delta(m)$ mean |
| minpeakheight | the minimum peak intensity |
| noiseacf | aytorelation of the noise |
| ppmPeakMinSep | the minimum distance between two peeks in ppm |
| daSeparation | the minimum distance between two peeks in da |
| d | the degree of savitzky golay filter |
| plotAll | bollean if TRUE, it plot all the initialiation step |
| c | the number of current itteration |

Value

a list with fit input

LocalMaximaSG *Find local maxima with Savitzky Golay filter*

Description

Apply Savitzky Golay filter to the spectrum and find local maxima such that : second derivate Savitzky Golay filter < 0 and first derivate = 0 and intensity > minPeakHeight

Usage

```
LocalMaximaSG(sp, minPeakHeight = -Inf, noiseacf = 0.1, d = 3)
```

Arguments

sp the array of spectrum values
 minPeakHeight minimum intensity of a peak
 noiseacf autocorrelation of the noise
 d the degree of Savitzky Golay filter, default 3

Value

array with peak's index in the spectrum

Examples

```
spectrum<-dnorm(x=seq(-5,5,length.out = 100))
index.max<-LocalMaximaSG(spectrum)
```

makeSubGroup *Use in align function. return a peak group thanks to kernel gaussian density in a peak matrix.*

Description

Use in align function. return a peak group thanks to kernel gaussian density in a peak matrix.

Usage

```
makeSubGroup(subpeak1, den, plim)
```

Arguments

subpeak1 a matrix with mz, ppb, background and group column.
 den the kernel gaussian density estimated on subpeak1
 plim the limit of a peak in the density of the group who will be formed

Value

the sub peakgroup

| | |
|------------------|---|
| OptimalWindowsSG | <i>Find optimal window's size for Savitzky Golay filter</i> |
|------------------|---|

Description

Find optimal window's size for Savitzky Golay filter

Usage

```
OptimalWindowsSG(sp, noiseacf, d = 3)
```

Arguments

| | |
|----------|-------------------------------------|
| sp | the array of spectrum values |
| noiseacf | autocorrelation of the noise |
| d | the degree of Savitzky Golay filter |

Value

the optimal size of Savitzky Golay filter's windows

| | |
|----------|---|
| PeakList | <i>Detection and quantification of peaks on a sum spectrum.</i> |
|----------|---|

Description

Detection and quantification of peaks on a sum spectrum.

Usage

```
PeakList(
  raw,
  mzNominal = unique(round(getRawInfo(raw)$mz)),
  ppm = 130,
  resolutionRange = c(3000, 5000, 8000),
  minIntensity = 5,
  fctFit = c("sech2", "averagePeak")[1],
  peakShape = NULL,
  maxIter = 1,
  R2min = 0.995,
  autocorNoiseMax = 0.3,
  plotFinal = FALSE,
```

```

plotAll = FALSE,
thNoiseRate = 1.1,
minIntensityRate = 0.01,
countFacFWHM = 10,
daSeparation = 0.005,
d = 3,
windowSize = 0.4
)

## S4 method for signature 'ptrRaw'
PeakList(
  raw,
  mzNominal = unique(round(getRawInfo(raw)$mz)),
  ppm = 130,
  resolutionRange = c(300, 5000, 8000),
  minIntensity = 5,
  fctFit = c("sech2", "averagePeak")[1],
  peakShape = NULL,
  maxIter = 3,
  R2min = 0.995,
  autocorNoiseMax = 0.3,
  plotFinal = FALSE,
  plotAll = FALSE,
  thNoiseRate = 1.1,
  minIntensityRate = 0.01,
  countFacFWHM = 10,
  daSeparation = 0.005,
  d = 3,
  windowSize = 0.4
)

```

Arguments

| | |
|-----------------|---|
| raw | ptrRaw-class object |
| mzNominal | the vector of nominal mass where peaks will be detected |
| ppm | the minimum distance between two peaks in ppm |
| resolutionRange | vector with resolution min, resolution Mean, and resolution max of the PTR |
| minIntensity | the minimum intensity for peaks detection. The final threshold for peak detection will be : $\max(\text{minPeakDetect}, \text{thresholdNoise})$. The threshold-Noise correspond to $\max(\text{thNoiseRate} * \max(\text{noise around the nominal mass}), \text{minIntensityRate} * \max(\text{intensity in the nominal mass}))$. The noise around the nominal mass correspond : $[m-\text{windowSize}-0.2, m-\text{windowSize}] \cup [m+\text{windowSize}, m+\text{windowSize}+0.2]$ |
| fctFit | the function for the quantification of Peak, should be average or Sech2 |
| peakShape | a list with reference axis and a reference peak shape centered in zero |
| maxIter | maximum iteration of residual analysis |
| R2min | R2 minimum to stop the iterative residual analysis |

| | |
|------------------|---|
| autocorNoiseMax | the autocorrelation threshold for Optimal windows Savitzky Golay filter in OptimalWindowSG ptairMS function. See ?OptimalWindowSG |
| plotFinal | boolean. If TRUE, plot the spectrum for all nominal masses, with the final fitted peaks |
| plotAll | boolean. If TRUE, plot all step to get the final fitted peaks |
| thNoiseRate | The rate which multiplies the max noise intensity |
| minIntensityRate | The rate which multiplies the max signal intensity |
| countFacFWHM | integer. We will sum the fitted peaks on a window's size of countFacFWHM * FWHM, centered in the mass peak center. |
| daSeparation | the minimum distance between two peaks in Da for nominal mass < 17. |
| d | the degree for the Savitzky Golay filter |
| windowSize | peaks will be detected only around $m - \text{windowSize}$; $m + \text{windowSize}$, for all m in $mzNominal$ |

Value

a list containing:

- peak: a data.frame, with for all peak detected: the mass center, the intensity count in cps, the peak width (delta_mz), correspond to the Full Width Half Maximum (FWHM), the resolution m/delta_m , the other parameters values estimated of fitFunc.
- warnings: warnings generated by the peak detection algorithm per nominal masses
- infoPlot: elements needed to plot the fitted peak per nominal masses

Examples

```
library(ptairData)
filePath <- system.file('extdata/exhaledAir/ind1', 'ind1-1.h5',
  package = 'ptairData')
file <- readRaw(filePath)

peakList <- PeakList(file, mzNominal = c(21,63))
peakList$peak
```

plot,ptrSet,ANY-method

Plot a ptrSet object

Description

plot a ptrSet object

Usage

```
## S4 method for signature 'ptrSet,ANY'
plot(x, y, typePlot = "")
```

Arguments

| | |
|----------|---|
| x | a ptrSet object |
| y | not use |
| typePlot | could be : calibError, resolution, peakShape, or a empty character if you want all. |

Value

plot

Examples

```
dirRaw <- system.file("extdata/exhaledAir", package = "ptairData")
exhaledPtrset <- createPtrSet(dir=dirRaw, setName="exhaledPtrset",
mzCalibRef = c(21.022, 60.0525), fracMaxTIC = 0.7, saveDir = NULL )
plot(exhaledPtrset )
plot(exhaledPtrset ,typePlot='calibError')
plot(exhaledPtrset ,typePlot='resolution')
plot(exhaledPtrset ,typePlot='peakShape')
```

plotCalib

Plot the calibration peaks after calibration

Description

Plot the calibration peaks after calibration

Usage

```
plotCalib(object, ppm = 2000, ...)

## S4 method for signature 'ptrRaw'
plotCalib(object, ppm = 2000, ...)

## S4 method for signature 'ptrSet'
plotCalib(object, ppm = 2000, pdfFile = NULL, fileNames = NULL, ...)
```

Arguments

| | |
|-----------|--|
| object | a ptrSet or ptrRaw object |
| ppm | the width of plot windows |
| ... | not used |
| pdfFile | is different of NULL, the file path to save the plots in pdf |
| fileNames | the name of the files in the ptrSet object to plot. If NULL, all files will be plotted |

Value

plot

Examples

```
## ptrSet
dirRaw <- system.file("extdata/exhaledAir", package = "ptairData")
exhaledPtrset <- createPtrSet(dir=dirRaw, setName="exhaledPtrset",
mzCalibRef = c(21.022, 60.0525), fracMaxTIC = 0.7, saveDir = NULL )
plotCalib(exhaledPtrset ,fileNames=getFileNames(exhaledPtrset )[1])

## ptrRaw
filePath<-system.file('extdata/exhaledAir/ind1/ind1-1.h5',
package = 'ptairData')
raw <- readRaw(filePath,mzCalibRef=c(21.022,59.049))
plotCalib(raw)
```

plotFeatures

Plot raw average spectrum around a mzRange

Description

Plot the raw data spectrum for several files in a ptrSet object around the mz masses. The expiration average spectrum is in full lines, and background in dashed lines.

Usage

```
plotFeatures(
  set,
  mz,
  typePlot = "plotly",
  addFeatureLine = TRUE,
  ppm = 2000,
  pdfFile = NULL,
  fileNames = NULL,
  colorBy = "rownames"
)
```

```
## S4 method for signature 'ptrSet'
plotFeatures(
  set,
  mz,
  typePlot = "plotly",
  addFeatureLine = TRUE,
  ppm = 2000,
  pdfFile = NULL,
  fileNames = NULL,
  colorBy = "rownames"
)
```

Arguments

| | |
|----------------|--|
| set | a <code>ptrSet-class</code> object |
| mz | the mz values to plot |
| typePlot | set "plotly" to get an interactive plot, or "ggplot" |
| addFeatureLine | boolean. If TRUE a vertical line at the mz masses is plotted |
| ppm | windows size of the plot round mz in ppm |
| pdfFile | a file path to save a pdf with a individual plot per file |
| fileNames | vector of character. The file names you want to plot. If NULL, it plot all files |
| colorBy | character. A column name of sample metadata by which the line are colored. |

Value

a plotly or ggplot2 object

Examples

```
dirRaw <- system.file("extdata/exhaledAir", package = "ptairData")
exhaledPtrset <- createPtrSet(dir=dirRaw,
  setName="exhaledPtrset", mzCalibRef = c(21.022, 60.0525),
  fracMaxTIC = 0.7, saveDir = NULL )
plotF<-plotFeatures(exhaledPtrset ,mz=59.049,type="ggplot",colorBy="subfolder")
print(plotF)
```

| | |
|---------------|---|
| plotPeakShape | <i>plot the average peak shape of reference calibration masses for a ptrSet</i> |
|---------------|---|

Description

plot the average peak shape of reference calibration masses for a ptrSet

Usage

```
plotPeakShape(set, showAverage = FALSE)
```

Arguments

set ptrSet object
showAverage boolean

Value

ggplot object

plotRaw *Plot method for 'ptrRaw' objects*

Description

Displays the image of the matrix of intensities, the TIC and the TIS, for the selected m/z and time ranges

Usage

```
plotRaw(  
  object,  
  mzRange,  
  timeRange = c(NA, NA),  
  type = c("classical", "plotly")[1],  
  ppm = 2000,  
  palette = c("heat", "revHeat", "grey", "revGrey", "ramp")[1],  
  showVocDB = TRUE,  
  figure.pdf = "interactive",  
  ...  
)  
  
## S4 method for signature 'ptrRaw'  
plotRaw(  
  object,  
  mzRange,  
  timeRange = c(NA, NA),  
  type = c("classical", "plotly")[1],  
  ppm = 2000,  
  palette = c("heat", "revHeat", "grey", "revGrey", "ramp")[1],  
  showVocDB = TRUE,  
  figure.pdf = "interactive",  
  ...  
)  
  
## S4 method for signature 'ptrSet'  
plotRaw(  
  object,
```

```

mzRange,
timeRange = c(NA, NA),
type = c("classical", "plotly")[1],
ppm = 2000,
palette = c("heat", "revHeat", "grey", "revGrey", "ramp")[1],
showVocDB = TRUE,
figure.pdf = "interactive",
fileNames = NULL,
...
)

```

Arguments

| | |
|------------|---|
| object | An S4 object of class ptrRaw-class or ptrSet |
| mzRange | Either a vector of 2 numerics indicating the m/z limits or an integer giving a nominal m/z |
| timeRange | Vector of 2 numerics giving the time limits |
| type | Character: plot type; either 'classical' [default] or 'plotly' |
| ppm | Integer: Half size of the m/z window when mzRange is set to a nominal mass |
| palette | Character: Color palette for the 'classical' plot; either 'heat' [default], 'revHeat', 'grey', 'revGrey' or 'ramp' |
| showVocDB | Logical: Should putative m/z annotations from the internal package database be displayed (default is TRUE) |
| figure.pdf | Character: Either 'interactive' [default], or the filename of the figure to be saved (with the 'pdf' extension); only available for the 'classical' display |
| ... | not used |
| fileNames | vector of character. The file names of the ptrSer that you want to plot. Could be in basename or fullname. |

Value

Invisibly returns a list of the raw (sub)matrix 'rawsubM' and the voc (sub)database 'vocsubDB'

Examples

```

dirRaw <- system.file("extdata/exhaledAir", package = "ptairData")
exhaledPtrset <- createPtrSet(dir=dirRaw, setName="exhaledPtrset",
mzCalibRef = c(21.022, 60.0525), fracMaxTIC = 0.7, saveDir = NULL )
ptairMS::plotRaw(exhaledPtrset ,mzRange=59,fileNames='ind1-1.h5')

patientRaw <- ptairMS::readRaw(system.file('extdata/exhaledAir/ind1/ind1-1.h5',
package = 'ptairData'), mzCalibRef=c(21.022,59.049,75.05))
ptairMS::plotRaw(patientRaw, mzRange = 59)
ptairMS::plotRaw(patientRaw, mzRange = 59, type = 'plotly')

```

plotTIC *plot the Total Ion spectrum (TIC) for one or several files.*

Description

plot the Total Ion spectrum (TIC) for one or several files.

Usage

```
plotTIC(
  object,
  type = c("plotly", "ggplot")[1],
  baselineRm = FALSE,
  showLimits = FALSE,
  ...
)

## S4 method for signature 'ptrRaw'
plotTIC(object, type, baselineRm, showLimits, fracMaxTIC = 0.8, ...)

## S4 method for signature 'ptrSet'
plotTIC(
  object,
  type,
  baselineRm,
  showLimits,
  pdfFile = NULL,
  fileNames = NULL,
  colorBy = "rownames",
  normalizePrimariIon = FALSE,
  ...
)
```

Arguments

| | |
|------------|--|
| object | ptrSet or ptrRaw S4 object |
| type | set 'plotly' to get an interactive plot, and 'ggplot' for classical plot. |
| baselineRm | logical. If TRUE, remove the baseline of the TIC |
| showLimits | logical. If TRUE, add the time limits to the plot (obtain with the 'fracMaxTIC' argument or 'createPtrSet' function) |
| ... | not used |
| fracMaxTIC | Percentage (between 0 and 1) of the maximum of the Total Ion Current (TIC) amplitude with baseline removal. We will analyze only the part of the spectrum where the TIC intensity is higher than 'fracMaxTIC * max(TIC)'. If you want to analyze the entire spectrum, set this parameter to 0. |

| | |
|---------------------|---|
| pdfFile | a absolute file path. A pdf will be generated with a plot for each file, caints TIC and time limits. |
| fileNames | vector of character. The file names of the ptrSer that you want to plot. Could be in basename or fullname. |
| colorBy | character. A name of the ptrSet's sampleMetaData column, to display with the same color files of same attributes. |
| normalizePrimariIon | should the TIC be normalized by the primary ion |

Value

a plotly of ggplot2 object.

Examples

```
### ptrRaw object

library(ptairData)
filePath <- system.file('extdata/exhaledAir/ind1', 'ind1-1.h5',
package = 'ptairData')
raw <- readRaw(filePath)
p <- plotTIC(raw)
p
dirRaw <- system.file("extdata/exhaledAir", package = "ptairData")
exhaledPtrset <- createPtrSet(dir=dirRaw, setName="exhaledPtrset",
mzCalibRef = c(21.022, 60.0525), fracMaxTIC = 0.7, saveDir = NULL )
plotTIC(exhaledPtrset ,type='ggplot')
```

ptrRaw-class

PTR-TOF-MS raw data from a rhdf5 file

Description

A ptrRaw object contains PTR-TOF-MS raw data from one rhdf5 file. It is created with the [readRaw](#) function.

Slots

name the file name
rawM the raw intensities matrix
mz array of the m/z axis
time numeric vector of acquisition time (in seconds)
calibMzToTof function to convert m/z to Tof
calibTofToMz function to convert tof to m/z
calibCoef calibration coefficients (a,b) such that: $mz = ((tof-b)/a)^2$ for each calibration period
indexTimeCalib index time of each calibration period

calibMassRef the reference masses used for the calibration
 calibError the shift error in ppm at the reference masses
 calibSpectr the spectrum of calibration reference masses
 peakShape average normalized peak shape of the calibration peak
 ptrTransmisison matrix with transmission values
 prtReaction a list containing PTR reaction information: drift temperature, pressure and voltage
 date acquisition date and hour
 peakList individual peak list in [eSet](#)
 fctFit the peak function used for peak deconvolution for each file
 resolution estimation of the resolution for each file based on the calibration reference masses
 primaryIon the quantity in count per acquisition time of the isotope of primary ion for each file

References

<https://www.hdfgroup.org>

ptrSet-class

A set of PTR-TOF-MS raw data informations

Description

A ptrSet object is related to a directory that contains several PTR-TOF-MS raw data in rhdf5 format. It is created with the [createPtrSet](#) function. This object could be updated when new files are added with the [updatePtrSet](#) function.

Slots

parameter the input parameters value of the function [createPtrSet](#) and [detectPeak](#)
 sampleMetadata dataframe of sample metadata, with file names in row names, suborders names and acquisition date in columns
 date acquisition date for each file
 mzCalibRef the masses used for calibration for each file
 signalCalibRef the spectrum of mass calibration for each file
 errorCalibPpm the calibration error for each file
 coefCalib the coefficients of mass axis calibration of each calibration periods for each file
 indexTimeCalib index time of each calibration period for each file
 primaryIon the quantity in count per acquisition time of the isotope of primary ion for each file
 resolution estimation of the resolution for each file based on the calibration reference masses
 prtReaction drift information (temperature, pressure and voltage)
 ptrTransmisison transmission curve for each file

TIC the total ion current (TIC) for each file
 breathTracer the tracer for expiration/head spaces detection
 timeLimit the index of time limit for each file
 knots numeric vector correspond to the knot that will be used for the two dimensional regression for each file
 fctFit the peak function used for peak deconvolution for each file
 peakShape average normalized peak shape of the calibration peak for each file
 peakList individual peak list in [eSet](#)

| | |
|---------|--|
| readRaw | <i>Read a h5 file of PTR-TOF-MS data</i> |
|---------|--|

Description

readRaw reads a h5 file with rhdf5 library, and calibrates the mass axis with mzCalibRef masses each calibrationPeriod seconds. It returns a [ptrRaw-class](#) S4 object, that contains raw data.

Usage

```
readRaw(
  filePath,
  calib = TRUE,
  mzCalibRef = c(21.022, 29.013424, 41.03858, 60.0525, 203.943, 330.8495),
  calibrationPeriod = 60,
  tolCalibPpm = 70,
  maxTimePoint = 900
)
```

Arguments

| | |
|-------------------|--|
| filePath | h5 absolute file path full name. |
| calib | boolean. If true, an external calibration is performed on the calibrationPeriod sum spectrum with mzCalibRef reference masses. |
| mzCalibRef | calibration parameter. Vector of exact theoretical masses values of an intensive peak without overlapping. |
| calibrationPeriod | in second, coefficient calibration are estimated for each sum spectrum of calibrationPeriod seconds |
| tolCalibPpm | calibration parameter. The maximum error tolerated in ppm. A warning appears for error greater than tolCalibPpm. |
| maxTimePoint | number maximal of time point to read |

Value

a ptrRaw object, including slot

- rawM the data raw matrix, in count of ions
- mz the mz axis
- time time acquisition in second

Examples

```
library(ptairData)
filePathRaw <- system.file('extdata/exhaledAir/ind1', 'ind1-1.h5',
package = 'ptairData')
raw <- readRaw(filePathRaw, mzCalibRef=c(21.022, 60.0525), calib=FALSE)
```

| | |
|---------------------|---|
| resetSampleMetadata | <i>reset the default sampleMetadata, containing the suborders names and the acquisition dates as columns.</i> |
|---------------------|---|

Description

reset the default sampleMetadata, containing the suborders names and the acquisition dates as columns.

Usage

```
resetSampleMetadata(ptrset)
```

Arguments

ptrset a ptrser object

Value

a data.frame

Examples

```
dirRaw <- system.file("extdata/exhaledAir", package = "ptairData")
exhaledPtrset <- createPtrSet(dir=dirRaw, setName="exhaledPtrset",
mzCalibRef = c(21.022, 60.0525), fracMaxTIC = 0.7, saveDir = NULL )
SMD<- resetSampleMetadata(exhaledPtrset)
```

rmPeakList

remove the peakList of an ptrSet object

Description

This function is useful when you want to change the parameters of the detect peak function. First delete the peakList with rmPeakList, and apply detectPeakwith the new parameters.

Usage

```
rmPeakList(object)
```

Arguments

object ptrSet object

Value

a ptrSet

Examples

```
library(ptairData)
dirRaw <- system.file("extdata/exhaledAir", package = "ptairData")
exhaledPtrset <- createPtrSet(dir=dirRaw, setName="exhaledPtrset",
mzCalibRef = c(21.022, 60.0525), fracMaxTIC = 0.7, saveDir = NULL )
exhaledPtrset <-rmPeakList(exhaledPtrset )
```

RunShinnyApp*Graphical interface of ptairMS workflow*

Description

The whole workflow of ptairMS can be run interactively through a graphical user interface, which provides visualizations (expiration phases, peaks in the raw data, peak table, individual VOCs), quality controls (calibration, resolution, peak shape and evolution of reagent ions depending on time), and exploratory data analysis.

Usage

```
RunShinnyApp()
```

Value

Shinny app

Examples

```
## Not run: RunShinnyApp()
```

```
setSampleMetadata      set sampleMetadata in a ptrSet
```

Description

Insert a samplemetada data.frame in a ptrSet object. The dataframe must have all file names in rownames.

Usage

```
setSampleMetadata(set, sampleMetadata)
```

Arguments

```
set          a ptrSet object
sampleMetadata a data.frame with all file names of the ptrSet in row names
```

Value

the ptrSet object in argument with the sampleMetadata modified

Examples

```
dirRaw <- system.file("extdata/exhaledAir", package = "ptairData")
exhaledPtrset <- createPtrSet(dir=dirRaw, setName="exhaledPtrset",
mzCalibRef = c(21.022, 60.0525), fracMaxTIC = 0.7, saveDir = NULL )
SMD<-getSampleMetadata(exhaledPtrset )
colnames(SMD)[1]<-'individual'
exhaledPtrset<-setSampleMetadata(exhaledPtrset ,SMD)
```

```
show,ptrRaw-method      show a ptrRaw object
```

Description

It indicates the files, the mz range, time acquisition range, and calibration error.

Usage

```
## S4 method for signature 'ptrRaw'
show(object)
```

Arguments

object a ptrRaw object

Value

nothing

show, ptrSet-method *show a ptrSet object*

Description

It indicates the directory, the number of files that contain the directory at the moment, and the number of processed files. The two numbers are different, use updatePtrSet function.

Usage

```
## S4 method for signature 'ptrSet'
show(object)
```

Arguments

object a ptrSet object

Value

nothing

snipBase *Baseline estimation*

Description

Baseline estimation

Usage

```
snipBase(sp, widthI = 11, iteI = 5)
```

Arguments

sp an array with spectrum values
widthI width of interval
iteI number of iteration

Value

baseline estimation of the spectrum

`timeLimits`*Calculates time limits on the breath tracer*

Description

This function derives limits on the breath tracer indicated, where the intensity is greater than $\text{fracMaxTIC} \times \max(\text{tracer})$. By setting `fracMaxTIC` close to 1, the size of the limits will be restricted. This function also determine the index corresponding to the background, where variation between two successive point can be control with `derivThreshold` parameter.

Usage

```
timeLimits(  
  object,  
  fracMaxTIC = 0.5,  
  fracMaxTICBg = 0.2,  
  derivThresholdExp = 1,  
  derivThresholdBg = 0.05,  
  mzBreathTracer = NULL,  
  minPoints = 2,  
  degreeBaseline = 1,  
  baseline = TRUE,  
  redefineKnots = TRUE,  
  plotDel = FALSE  
)  
  
## S4 method for signature 'ptrRaw'  
timeLimits(  
  object,  
  fracMaxTIC = 0.6,  
  fracMaxTICBg = 0.2,  
  derivThresholdExp = 0.5,  
  derivThresholdBg = 0.05,  
  mzBreathTracer = NULL,  
  minPoints = 2,  
  degreeBaseline = 1,  
  baseline = TRUE,  
  redefineKnots = TRUE,  
  plotDel = FALSE  
)  
  
## S4 method for signature 'ptrSet'  
timeLimits(  
  object,  
  fracMaxTIC = 0.5,  
  fracMaxTICBg = 0.2,  
  derivThresholdExp = 1,
```

```

    derivThresholdBg = 0.05,
    minPoints = 2,
    degreeBaseline = 1,
    baseline = TRUE,
    redefineKnots = TRUE,
    plotDel = FALSE
  )

```

Arguments

| | |
|-------------------|---|
| object | a ptrRaw or ptrSet object |
| fracMaxTIC | between 0 and 1. Percentage of the maximum of the tracer amplitude with baseline removal. If you want a finer limitation, increase fracMaxTIC, indeed decrease |
| fracMaxTICBg | same as fracMaxTIC but for background detection (lower than fracMaxTIC*max(TIC)) |
| derivThresholdExp | the threshold of the difference between two successive points of the expiration |
| derivThresholdBg | the threshold of the difference between two successive points of the background |
| mzBreathTracer | NULL or a integer. Correspond to a nominal masses of Extract Ion Current (EIC) whose limits you want to compute. If NULL, the limits are calculated on the Total Ion Current (TIC). |
| minPoints | minimum duration of an expiration (in index). |
| degreeBaseline | the degree of polynomial baseline function |
| baseline | logical, should the trace be baseline corrected? |
| redefineKnots | logical, should the knot location must be redefined with the new times limits ? |
| plotDel | boolean. If TRUE, the trace is plotted with limits and threshold. |

Value

a list with expiration limits (a matrix of index, where each column correspond to one expiration, the first row it is the beginning and the second the end, or NA if no limits are detected) and index of the background.

Examples

```

## ptrRaw object

library(ptairData)
filePath <- system.file('extdata/exhaledAir/ind1', 'ind1-1.h5',
  package = 'ptairData')
raw <- readRaw(filePath)

timLim <- timeLimits(raw, fracMaxTIC=0.9, plotDel=TRUE)
timLim_acetone <- timeLimits(raw, fracMaxTIC=0.5, mzBreathTracer = 59,
  plotDel=TRUE)

```

| | |
|-------------------|--|
| TransmissionCurve | <i>Estimation of the transmissison curve</i> |
|-------------------|--|

Description

Estimation of the transmissison curve

Usage

TransmissionCurve(x, y)

Arguments

| | |
|---|-------------------|
| x | masses |
| y | transmission data |

Value

a numeric vector

| | |
|--------------|-------------------------------|
| updatePtrSet | <i>update a ptrSet object</i> |
|--------------|-------------------------------|

Description

When new files are added to a directory which has already a ptrSet object associated, run updatePtrSet to add the new files in the object. The information on the new files are added to object with the same parameter used for the function createPtrSet who has created the object. updatePtrSet also delete from the ptrSet deleted files in the directory.

Usage

updatePtrSet(ptrset)

Arguments

| | |
|--------|-----------------|
| ptrset | a ptrset object |
|--------|-----------------|

Value

teh same ptrset object than ininput, but completed with new files and without deleted files in the directory

Examples

```
dirRaw <- system.file("extdata/exhaledAir", package = "ptairData")
exhaledPtrset <- createPtrSet(dir=dirRaw, setName="exhaledPtrset",
mzCalibRef = c(21.022, 60.0525), fracMaxTIC = 0.7, saveDir = NULL )
##add or delete files in the directory
# exhaledPtrset<- updatePtrSet(exhaledPtrset)
```

| | |
|-------|--|
| width | <i>Calculate the FWHM (Full Width at Half Maximum) in raw data</i> |
|-------|--|

Description

Calculate the FWHM (Full Width at Half Maximum) in raw data

Usage

```
width(tof, peak, fracMaxTIC = 0.5)
```

Arguments

| | |
|------------|--|
| tof | A vector of tof interval |
| peak | A vector of peak Intensity |
| fracMaxTIC | the fraction of the maximum intenisty to compute the width |

Value

the delta FWHM in tof

| | |
|-----------|--|
| writeEset | <i>Exporting an ExpressionSet instance into 3 tabulated files 'dataMatrix.tsv', 'sampleMetadata.tsv', and 'variableMetadata.tsv'</i> |
|-----------|--|

Description

Note that the dataMatrix is transposed before export (e.g., the samples are written column wise in the 'dataMatrix.tsv' exported file).

Usage

```
writeEset(x, dirName, overwrite = FALSE, verbose = TRUE)

## S4 method for signature 'ExpressionSet'
writeEset(x, dirName, overwrite = FALSE, verbose = TRUE)
```

Arguments

| | |
|-----------|---|
| x | An S4 object of class ExpressionSet |
| dirName | Character: directory where the tables should be written |
| overwrite | Logical: should existing files be overwritten? |
| verbose | Logical: should messages be printed? |

Value

No object returned.

Examples

```
library(ptairData)
dirRaw <- system.file("extdata/exhaledAir", package = "ptairData")
exhaledPtrset <- createPtrSet(dir=dirRaw, setName="exhaledPtrset",
mzCalibRef = c(21.022, 60.0525), fracMaxTIC = 0.7, saveDir = NULL )
exhaledPtrset<-detectPeak(exhaledPtrset,mz=c(21,59,77))
eset <- ptairMS::alignSamples(exhaledPtrset )
writeEset(eset, dirName = file.path(getwd(), "processed_dataset"))
unlink(file.path(getwd(), "processed_dataset"),recursive = TRUE)
```

Index

* internal

- align, 4
 - calibrationFun, 10
 - cumulative_fit_function, 14
 - deadTimeCorr, 15
 - determinePeakShape, 20
 - extractEIC, 21
 - fit_averagePeak, 21
 - fit_averagePeak_function, 22
 - initializeFit, 28
 - makeSubGroup, 30
 - OptimalWindowsSG, 31
 - plotPeakShape, 36
 - ptairMS-package, 3
 - snipBase, 46
 - TransmissionCurve, 49
 - width, 50
- aggregate, 4
- align, 4
- alignSamples, 5, 27
- alignSamples, ptrSet-method
(alignSamples), 5
- annotateVOC, 7
- annotateVOC, data.frame-method
(annotateVOC), 7
- annotateVOC, ExpressionSet-method
(annotateVOC), 7
- annotateVOC, numeric-method
(annotateVOC), 7
- calibration, 9, 13
- calibration, ptrRaw-method
(calibration), 9
- calibration, ptrSet-method
(calibration), 9
- calibrationFun, 10
- changeTimeLimits, 11
- convert_to_mzML, 11
- createPtrSet, 12, 41
- cumulative_fit_function, 14
- deadTimeCorr, 15
- defineKnots, 15, 19
- defineKnots, ptrRaw-method
(defineKnots), 15
- defineKnots, ptrSet-method
(defineKnots), 15
- detectPeak, 6, 12, 17, 27, 41
- detectPeak, ptrRaw-method (detectPeak),
17
- detectPeak, ptrSet-method (detectPeak),
17
- determinePeakShape, 20
- eSet, 14, 41, 42
- exportSampleMetada, 20
- ExpressionSet, 5, 6
- extractEIC, 21
- fit_averagePeak, 21
- fit_averagePeak_function, 22
- formula2mass, 23
- getDirectory, 23
- getFileNames, 24
- getFileNames, ptrRaw-method
(getFileNames), 24
- getFileNames, ptrSet-method
(getFileNames), 24
- getPeakList, 14, 17, 25
- getSampleMetadata, 26
- importSampleMetadata, 26
- impute, 27
- imputeMat, 28
- initializeFit, 28
- LocalMaximaSG, 30
- makeSubGroup, 30

OptimalWindowsSG, 31

PeakList, 31

PeakList, ptrRaw-method (PeakList), 31

plot, ptrSet, ANY-method, 33

plot, ptrSet-method
 (plot, ptrSet, ANY-method), 33

plot.ptrSet (plot, ptrSet, ANY-method), 33

plotCalib, 34

plotCalib, ptrRaw-method (plotCalib), 34

plotCalib, ptrSet-method (plotCalib), 34

plotFeatures, 35

plotFeatures, ptrSet-method
 (plotFeatures), 35

plotPeakShape, 36

plotRaw, 37

plotRaw, ptrRaw-method (plotRaw), 37

plotRaw, ptrSet-method (plotRaw), 37

plotTIC, 39

plotTIC, ptrRaw-method (plotTIC), 39

plotTIC, ptrSet-method (plotTIC), 39

ptairMS (ptairMS-package), 3

ptairMS-package, 3

ptrRaw-class, 40

ptrSet, 18

ptrSet-class, 41

readRaw, 40, 42

resetSampleMetadata, 43

rmPeakList, 44

RunShinnyApp, 44

setSampleMetadata, 45

show, ptrRaw-method, 45

show, ptrSet-method, 46

snipBase, 46

timeLimits, 14, 19, 47

timeLimits, ptrRaw-method (timeLimits),
 47

timeLimits, ptrSet-method (timeLimits),
 47

TransmissionCurve, 49

updatePtrSet, 41, 49

width, 50

writeEset, 50

writeEset, ExpressionSet-method
 (writeEset), 50