Package 'ptairMS'

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Title Pre-processing PTR-TOF-MS Data

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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 singl<e 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 identfy four potentiel biomarquers of the infection.

License GPL-3

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

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`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 singl<e 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 identfy four potentiel biomarquers of the infection.

Author(s)

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See Also

Useful links:

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

aggregate *aggregate peakgroup for align function*

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 *Alignment with kernel gaussian density*

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 — *Putative annotation of VOC mz by using the reference compilation from the literature*

Description

Putatively annotate VOC mz by using the reference compilation from the literature, and porpose an isotope detetcion.

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	Characer 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

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

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`	coeficient of the previous calibration
`peakShape`	a list with reference axis and a reference peak shape centered in zero
`tol`	maximum error tolarated in ppm

Value

list

`changeTimeLimits` *Shinny appplication 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.*

Description

Shinny appplication 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 *Convert a h5 file to mzML*

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 *Creates a ptrSet object form a directory*

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 *Dead time correction on raw data*

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 *Define the knots location*

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 ptrSet object
ppm	minimum distance in ppm between two peaks
minIntensity	minimum intensity for peak detection. The final threshold for peak detection will be: max(minIntensity, threshold noise). The threshold noise corresponds to max(max(noise around the nominal mass), minIntensityRate * max(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 sech2 or averagePeak. 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 descibe by average and al 2013, for determine a peak shape from the raw data :
$peak_i(Delta_i,A_i,t_i) = interpolation(x= tof.ref * Delta_i + t_i,y = A_i * peak.ref, xout= TOF_i)$ 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 *extract all raw EIC from a pre-definied peak List*

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` *Fit peak with average function*

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 *Compute exact mass.*

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 *get the files directory of a ptrSet*

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

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 *get the peak list of a ptrSet object*

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 metada to import, with all file names in row name (the fist column on th excel).

Value

a ptrSet with th enew 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 *Impute missing values on an matrix set from an ptrSet*

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` *initialization for apply fit function in the spectrum*

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 fetted (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`	aytocorelation 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, defalut 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(subpeakl, den, plim)
```

Arguments

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

Value

the sub peakgroup

OptimalWindowsSG *Find optimal window's size for Savitzky Golay filter*

Description

Find optimal window's size for Savitzky Golay filter

Usage

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

Arguments

sp	the array of specrtum values
noiseacf	autocorrelation of the noise
d	the degree of Savitzky Golay filter

Value

the optimal size of Savitzky Golay filter's windows

PeakList *Detection and quantification of peaks on a sum spectrum.*

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 peeks in ppm
resolutionRange	vector with resolution min, resolution Mean, and resolution max of the PTR
minIntensity	the minimum intenisty for peaks detection. The final threshold for peak detection will be : max (minPeakDetect , thresholdNoise). The thresholdNoise correspond to max(thNoiseRate * max(noise around the nominal mass), minIntensityRate * max(intenisty in the nominal mass). The noise around the nominal mass correspond : [m-windowSize-0.2,m-windowSize]U[m+windowSize,m+WindowSize+
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 autocorelation 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. Tf 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 peeks in Da for nominal mass < 17.
d	the degree for the Savitzky Golay filtrer
windowSize	peaks will be detected only around m - windowSize ; m + 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 ptrSet-class 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` *plot the average peak shape of reference calibration masses for a ptrSet*

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 sptectrum (TIC) for one or several files.*

Description

plot the Total Ion sptectrum (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` *Read a h5 file of PTR-TOF-MS data*

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(filePath=filePathRaw, mzCalibRef=c(21.022, 60.0525), calib=FALSE)
```

---

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

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 `detectPeak`with 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 numbre 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 `fracMaxTIC*max(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 *Estimation of the transmisison curve*

Description

Estimation of the transmisison curve

Usage

```
TransmissionCurve(x, y)
```

Arguments

x	masses
y	transmission data

Value

a numeric vector

---

updatePtrSet *update a ptrSet object*

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

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 — *Exporting an ExpressionSet instance into 3 tabulated files 'dataMatrix.tsv', sampleMetadata.tsv', and 'variableMetadata.tsv'*

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)
```

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