Package 'msPurity'

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Type Package

Title Automated Evaluation of Precursor Ion Purity for Mass Spectrometry Based Fragmentation in Metabolomics

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Description Assess the contribution of the targeted precursor in fragmentation acquired or anticipated isolation windows using a metric called ``precursor purity''. Also provides simple processing steps (averaging, filtering, blank subtraction, etc) for DI-MS data. Works for both LC-MS(/MS) and DI-MS(/MS) data. Spectral matching of fragmentation spectra can also be run against a SQLite database of library spectra.

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assessPuritySingle . . . 2
averageSpectra,purityD-method . . . 3
averageSpectraSingle . . . 5
create_database . . . 6
dimsPredictPurity,purityD-method . . . 7
dimsPredictPuritySingle . . . 8
filterp,purityD-method . . . 9
frag4feature,purityA-method . . . 10
Getfiles . . . 11
getP,purityD-method . . . 11
get_additional_mzml_meta . . . 12
groupPeaks,purityD-method . . . 13
groupPeaksEx . . . 13
initialize,purityD-method . . . 14
iwNormGauss . . . 15
iwNormQE.5 . . . 16
iwNormRcosine . . . 16
pcalc . . . 17
purityA . . . 18
purityD-class . . . 19
purityX . . . 20
show,purityA-method . . . 21
show,purityD-method . . . 22
show,purityX-method . . . 22
spectral_matching . . . 23
subtract,purityD-method . . . 24
subtractMZ . . . 25
validate,purityA-method . . . 26
writeOut,purityD-method . . . 26

Index **27**

`assessPuritySingle` *Assess the purity of a single LC-MS/MS or DI-MS/MS file*

Description

Given a filepath to an mzML file the precursor purity for any MS/MS scans will be outputed into a dataframe

Usage

```
assessPuritySingle(filepth, fileid = NA, mostIntense = FALSE,
  nearest = TRUE, offsets = NA, cores = 1, plotP = FALSE,
  plotdir = NULL, interpol = "linear", iwNorm = FALSE, iwNormFun = NULL,
  ilim = 0, mzRback = "pwiz", isotopes = TRUE, im = NULL)
```

Arguments

filepth	character; mzML file path for MS/MS spectra
fileid	numeric; adds a fileid column (primarily for internal use for msPurity)
mostIntense	boolean; True if the most intense peak is used for calculation. False if the centered peak is used
nearest	boolean; True if the peak selected is as the nearest MS1 scan. If False then the preceding scan is used
offsets	vector; Overide the isolation offsets found in the mzML filee.g. c(0.5, 0.5)
cores	numeric; Number of cores to use
plotP	boolean; If TRUE a plot of the purity is to be saved
plotdir	vector; If plotP is TRUE plots will be saved to this directory
interpol	character; Type of interolation to be performed "linear", "spline" or "none"
iwNorm	boolean; If TRUE then the intensity of the isolation window will be normalised based on the iwNormFun function
iwNormFun	function; A function to normalise the isolation window intensity. The default function is very generalised and just accounts for edge effects
ilim	numeric; All peaks less than this percentage of the target peak will be removed from the purity calculation, default is 5% (0.05)
mzRback	character; Backend to use for mzR parsing
isotopes	boolean; TRUE if isotopes are to be removed
im	matrix; Isotope matrix, default removes C13 isotopes (single, double and triple bonds)

Value

a dataframe of the purity score of the ms/ms spectra

See Also

purityA

Examples

```
filepth <- system.file("extdata", "lcms", "mzML", "LCMSMS_1.mzML", package="msPurityData")

puritydf <- assessPuritySingle(filepth)
```

---

averageSpectra,purityD-method

Using purityD object, calculates to average mz, intensity and signal-to-noise of multiple scans from multiple MS datafiles (mzML or .csv)

Description

Uses a purityD object with references to multiple MS files. For each file: Averages multiple scans together, see averageSpectraSingle for more information

Usage

```
## S4 method for signature 'purityD'
averageSpectra(Object, rtscn = "all", scanRange = NA,
  timeRange = NA, clustType = "hc", ppm = 1.5, snthr = 3,
  av = "median", missingV = "zero", minfrac = 0.6667, normTIC = FALSE,
  snMeth = "median")
```

Arguments

Object	object; purityD object
rtscn	character; Whether it is scans or retention time to be filtered. Use "all" if all scans to be used. ['rt', 'scns', 'all']
scanRange	vector; Scan range (if rtscn='scns') e.g. c(40, 69)
timeRange	vector; Time range (if rtscn='rt) e.g. c(10.3, 400.8) (only if using mzML file)
clustType	character; Type of clustering used either Hierarchical or just simple 1D grouping ['hc', 'simple']
ppm	numeric; The ppm error to cluster mz together
snthr	numeric; Signal to noise ratio threshold
av	character; What type of averaging to do between peaks
missingV	character; What to do with missing values (zero or ignore)
minfrac	numeric; Min fraction of scans with a grouped peak to be an accepted averaged peak
normTIC	boolean; If TRUE then RSD calculation will use the normalised intensity (intensity divided by TIC) if FALSE will use standard intensity
snMeth	character; Type of snMethod to use ['mean', 'median', 'precalc']. Precalc only applicable when using the csvFile parameter as TRUE

Value

purityD object with averaged spectra

See Also

averageSpectraSingle

Examples

```
datapth <- system.file("extdata", "dims", "mzML", package="msPurityData")
inDF <- Getfiles(datapth, pattern=".mzML", check = FALSE, cStrt = FALSE)
ppDIMS <- purityD(fileList=inDF, cores=1, mzML=TRUE)
ppDIMS <- averageSpectra(ppDIMS)
```

averageSpectraSingle *Calculates to average mz, intensity and signal-to-noise of multiple scans from 1 MS datafile (mzML or .csv)*

Description

Averages multiple scans of mass spectrometry data together. Each scan consisting of a minimum of intensity and mz values.

Works for either mzML or a .csv file consisting of mz, i, scanid, (optional: noise, backgroun, snr)

Signal-to-noise (SNR) can be calculated a number of ways. Default is to calculate the SN for every scan as the "Intensity of peak / the median intensity of the scan".

Alternatively if using a .csv file as input (and assigning the csvFile parameter to TRUE), a precalculated SNR can be one of the columns. The precalculated SNR can then be chosen by using the option 'precalc' for the parameter snMethod

The function will work for both LC-MS or DI-MS datasets.

Usage

```
averageSpectraSingle(filePth, rtscn = "all", scanRange = NA,
  timeRange = NA, clustType = "hc", ppm = 1.5, snthr = 3, cores = 1,
  av = "median", missingV = "ignore", minfrac = 0.6667,
  snMeth = "median", csvFile = FALSE, normTIC = FALSE, mzRback = "pwiz",
  MSFileReader = FALSE)
```

Arguments

filePth	character; Path of the file to be processed
rtscn	character; Whether it is scans or retention time to be filtered. Use "all" if all scans to be used. ['rt', 'scns', 'all']
scanRange	vector; Scan range (if rtscn='scns') e.g. c(40, 69)
timeRange	vector; Time range (if rtscn='rt) e.g. c(10.3, 400.8) (only if using mzML file)
clustType	character; Type of clustering used either Hierarchical or just simple 1D grouping ['hc', 'simple']
ppm	numeric; The ppm error to cluster mz together
snthr	numeric; Signal to noise ratio threshold
cores	numeric; Number of cores used to perform Hierarchical clustering WARNING: memory intensive, default 2
av	character; What type of averaging to do between peaks
missingV	character; What to do with missing values (zero or ignore)
minfrac	numeric; Min fraction of scans with a grouped peak to be an accepted averaged peak
snMeth	character; Type of snMethod to use ['mean', 'median', 'precalc']. Precalc only applicable when using the csvFile parameter as TRUE
csvFile	boolean; A csv file can be used as input. Useful for thermo files where the MSFileReader API can extract peaklist. This can consist of an .csv file with the following columns c('mz', 'i', 'scanid', 'snr')

normTIC	boolean; If TRUE then RSD calculation will use the normalised intensity (intensity divided by TIC) if FALSE will use standard intensity
mzRback	character; Backend to use for mzR parsing
MSFileReader	boolean; Deprecapted. Use csvFile parameter

Value

dataframe of the median mz, intensity, signal-to-noise ratio.

Examples

```
mzmlPth <- system.file("extdata", "dims", "mzML", "B02_Daph_TEST_pos.mzML", package="msPurityData")
avP <- averageSpectraSingle(mzmlPth)
```

---

create_database *Create database*

Description

Create and SQLite database of an LC-MS(/MS) experiment

Usage

```
create_database(pa, xset, xsa = NULL, out_dir, grp_peaklist = NA,
  db_name = NA)
```

Arguments

pa	purityA object; Needs to be the same used for frag4feature function
xset	xcms object; Needs to be the same used for frag4feature function (this will be ignored when using xsa parameter)
xsa	CAMERA object [optional]; if CAMERA object is used, we ignore the xset parameter input and obtain all information from the xset object nested with the CAMERA xsa object. Adduct and isotope information will be included into the database when using this parameter. The underlying xset object must be the one used for the frag4feature function
out_dir	character; Out directory for the SQLite result database
grp_peaklist	dataframe [optional]; Can use any peak dataframe. Still needs to be derived from the xset object though
db_name	character [optional]; Name of the result database

Value

path to SQLite database and database name

`dimsPredictPurity,purityD-method`
Using purityD object, assess anticipated purity from a DI-MS run

Description

Assess the precursor purity of anticpated MS/MS spectra. i.e. it 'predicts' the precursor purity of the DI-MS peaks for a future MS/MS run.

Usage

```
## S4 method for signature 'purityD'
dimsPredictPurity(Object, ppm = 1.5, minOffset = 0.5,
  maxOffset = 0.5, iwNorm = FALSE, iwNormFun = NULL, ilim = 0.05,
  sampleOnly = FALSE, isotopes = TRUE, im = NULL)
```

Arguments

`Object`	object = purityD object
`ppm`	numeric = tolerance for target mz value in each scan
`minOffset`	numeric = isolation window minimum offset
`maxOffset`	numeric = isolation window maximum offset
`iwNorm`	boolean = if TRUE then the intensity of the isolation window will be normalised based on the iwNormFun function
`iwNormFun`	function = A function to normalise the isolation window intensity. The default function is very generalised and just accounts for edge effects
`ilim`	numeric = All peaks less than this percentage of the target peak will be removed from the purity calculation, default is 5% (0.05)
`sampleOnly`	boolean = if TRUE will only calculate purity for sample peaklists
`isotopes`	boolean = TRUE if isotopes are to be removed
`im`	matrix = Isotope matrix, default removes C13 isotopes (single, double and triple bonds)

Value

purityD object with predicted purity of peaks

purityD object

See Also

`dimsPredictPuritySingle`

Examples

```
datapth <- system.file("extdata", "dims", "mzML", package="msPurityData")
inDF <- Getfiles(datapth, pattern=".mzML", check = FALSE, cStrt = FALSE)
ppDIMS <- purityD(fileList=inDF, cores=1, mzML=TRUE)
ppDIMS <- averageSpectra(ppDIMS)
ppDIMS <- filterp(ppDIMS)
ppDIMS <- subtract(ppDIMS)
ppDIMS <- dimsPredictPurity(ppDIMS)
```

`dimsPredictPuritySingle`

Predict the precursor purity from a DI-MS dataset

Description

Given a an DI-MS dataset (either mzML or .csv file) calculate the predicted purity for a vector of mz values.

Calculated at a given offset e.g. for 0.5 +/- Da the minOffset would be 0.5 and the maxOffset of 0.5.

A ppm tolerance is used to find the target mz value in each scan.

Usage

```
dimsPredictPuritySingle(mztargets, filepth, minOffset = 0.5,
  maxOffset = 0.5, ppm = 2.5, mzML = TRUE, iwNorm = FALSE,
  iwNormFun = NULL, ilim = 0.05, mzRback = "pwiz", isotopes = TRUE,
  im = NULL, sim = FALSE)
```

Arguments

`mztargets`	vector = mz targets to get predicted purity for
`filepth`	character = mzML file path or .csv file path
`minOffset`	numeric = isolation window minimum offset
`maxOffset`	numeric = isolation window maximum offset
`ppm`	numeric = tolerance for target mz value in each scan
`mzML`	boolean = Whether an mzML file is to be used or .csv file (TRUE == mzML)
`iwNorm`	boolean = if TRUE then the intensity of the isolation window will be normalised based on the iwNormFun function
`iwNormFun`	function = A function to normalise the isolation window intensity. The default function is very generalised and just accounts for edge effects
`ilim`	numeric = All peaks less than this percentage of the target peak will be removed from the purity calculation, default is 5% (0.05)
`mzRback`	character = backend to use for mzR parsing
`isotopes`	boolean = TRUE if isotopes are to be removed
`im`	matrix = Isotope matrix, default removes C13 isotopes (single, double and triple bonds)
`sim`	boolean = TRUE if file is from sim stitch experiment. Default FALSE

Value

a dataframe of the target mz values and the predicted purity score

Examples

```
mzmlPth <- system.file("extdata", "dims", "mzML", "B02_Daph_TEST_pos.mzML", package="msPurityData")
predicted <- dimsPredictPuritySingle(c(173.0806, 216.1045), filepth=mzmlPth , minOffset=0.5, maxOffset=0.5,
```

---

filterp,purityD-method

Filter out peaks based on intensity and RSD criteria

Description

Uses a purityD object remove peaks from either (or both) samples and blanks that are either below an intensity threshold or greater than a Relative Standard Deviation (RSD) threshold

Usage

```
## S4 method for signature 'purityD'
filterp(Object, thr = 5000, rsd = 20,
  sampleOnly = TRUE)
```

Arguments

Object	object; purityD object
thr	numeric; intensity threshold
rsd	numeric; rsd threshold
sampleOnly	boolean; if only the sample (not blanks) should be filtered

Value

purityD object

Examples

```
datapth <- system.file("extdata", "dims", "mzML", package="msPurityData")
inDF <- Getfiles(datapth, pattern=".mzML", check = FALSE, cStrt = FALSE)

ppDIMS <- purityD(inDF, cores=1)
ppDIMS <- averageSpectra(ppDIMS)
ppDIMS <- filterp(ppDIMS, thr = 5000)
```

`frag4feature,purityA-method`

Assign precursor purity scored fragmentation spectra to XCMS features

Description

Assign fragmentation spectra (MS/MS) scored via msPurity package to features from an XCMS set object.

Allows the user to filter out spectra below a certain threshold for purity.

Usage

```
## S4 method for signature 'purityA'
frag4feature(pa, xset, ppm = 5, plim = 0,
  intense = TRUE, convert2RawRT = TRUE, create_db = FALSE,
  out_dir = ".", db_name = NA, grp_peaklist = NA)
```

Arguments

pa	object; purityA object
xset	object; XCMS object derived from the same files as the puritydf
ppm	numeric; ppm tolerance between precursor mz and feature mz
plim	numeric; min purity of precursor to be included
intense	boolean; If the most intense precursor or the centered precursor is used
convert2RawRT	boolean; If retention time correction has been used in XCMS set this to TRUE
create_db	boolean; SQLite database will be created of the results
out_dir	character; Path where database will be created
db_name	character; If create_db is TRUE, a custom database name can be used, default is a time stamp
grp_peaklist	dataframe [optional]; Can use any peak dataframe to add to databse. Still needs to be derived from the xset object though

Value

purityA object with slots for fragmentation-XCMS links

Examples

```
msmsPths <- list.files(system.file("extdata", "lcms", "mzML", package="msPurityData"), full.names = TRUE, pa
xset <- xcms::xcmsSet(msmsPths, nSlaves = 1)
xset <- xcms::group(xset)
xset <- xcms::retcor(xset)
xset <- xcms::group(xset)

pa  <- purityA(msmsPths, interpol = "linear")
pa <- frag4feature(pa, xset)
```

Getfiles *Get files for DI-MS processing*

Description

Takes in a folder path and outputs the a data frame structure for purityD. Function modified from mzmatch.

Usage

```
Getfiles(projectFolder = NULL, recursive = FALSE, pattern = ".csv",
  check = TRUE, raw = FALSE, peakout = NA, cStrt = TRUE,
  mzml_out = FALSE)
```

Arguments

projectFolder	character; Directory path
recursive	boolean; Recursively check for files
pattern	character; File suffix to check for
check	boolean; Check with a GUI the files
raw	(REDUNDANT)
peakout	(REDUNDANT)
cStrt	boolean; Use the first word as the class name for files
mzml_out	(REDUNDANT)

Value

dataframe of files

Examples

```
datapth <- system.file("extdata", "dims", "mzML", package="msPurityData")
inDF <- Getfiles(datapth, pattern=".mzML", check = FALSE, cStrt = FALSE)
```

getP,purityD-method *Get peaklist for a purityD object*

Description

output peak list for a purityD object

Usage

```
## S4 method for signature 'purityD'
getP(x)
```

Arguments

x	object; purityD object

Value

peaks

Examples

```
datapth <- system.file("extdata", "dims", "mzML", package="msPurityData")
inDF <- Getfiles(datapth, pattern=".mzML", check = FALSE, cStrt = FALSE)
ppDIMS <- purityD(fileList=inDF, cores=1, mzML=TRUE)
peaks <- getP(ppDIMS)
```

---

get_additional_mzml_meta

Get additional mzML meta

Description

Extract the filter strings 'accession MS:1000512' from an mzML file. Called header in thermo software. Enables quick access to various information regarding each scan

Usage

```
get_additional_mzml_meta(mzml_pth)
```

Arguments

mzml_pth	character; mzML path

Value

dataframe of meta info

Examples

```
mzml_pth <- system.file("extdata", "dims", "mzML", 'B02_Daph_TEST_pos.mzML', package="msPurityData")
meta_df <- get_additional_mzml_meta(mzml_pth)
```

groupPeaks,purityD-method

Using purityD object, group multiple peaklists by similar mz values (mzML or .csv)

Description

Uses a purityD object to group all the peaklists in the 'avPeaks$processing' slot

Usage

```
## S4 method for signature 'purityD'
groupPeaks(Object, ppm = 3, sampleOnly = FALSE,
  clustType = "hc")
```

Arguments

Object	object = purityD object
ppm	numeric = The ppm tolerance to group peaklists
sampleOnly	= if TRUE the sample peaks will only be grouped
clustType	= if 'hc' the hierarchical clustering, if 'simple' the mz values will just be grouped using a simple 1D method

Value

data.frame of peaklists grouped together by mz

Examples

```
datapth <- system.file("extdata", "dims", "mzML", package="msPurityData")
inDF <- Getfiles(datapth, pattern=".mzML", check = FALSE, cStrt = FALSE)
ppDIMS <- purityD(fileList=inDF, cores=1, mzML=TRUE)
ppDIMS <- averageSpectra(ppDIMS)
grpedP <- groupPeaks(ppDIMS)
```

groupPeaksEx *Group peaklists from a list of dataframes*

Description

Group a list of dataframes by their m/z values

Usage

```
groupPeaksEx(peak_list, cores = 1, clustType = "hc", ppm = 2)
```

Arguments

peak_list	list = A list (named) of dataframes consiting of a least the following columns ['peakID', 'mz']
cores	= number of cores used for calculation
clustType	= if 'hc' the hierarchical clustering, if 'simple' the mz values will just be grouped using a simple 1D method
ppm	numeric = The ppm tolerance to group peaklists

Value

data.frame of peaklists grouped together by mz

Examples

```
datapth <- system.file("extdata", "dims", "mzML", package="msPurityData")
inDF <- Getfiles(datapth, pattern=".mzML", check = FALSE, cStrt = FALSE)
ppDIMS <- purityD(fileList=inDF, cores=1, mzML=TRUE)
ppDIMS <- averageSpectra(ppDIMS)
grpedP <- groupPeaks(ppDIMS)
```

---

initialize,purityD-method

Constructor for S4 class to represent a DI-MS purityD

Description

The class used to predict purity from an DI-MS dataset.

Usage

```
## S4 method for signature 'purityD'
initialize(.Object, fileList, cores = 1, mzML = TRUE,
  mzRback = "pwiz")
```

Arguments

.Object	object; purityD object
fileList	data.frame; created using GetFiles, data.frame with filepaths and sample class information
cores	numeric; Number of cores used to perform Hierarchical clustering WARNING: memory intensive, default 1
mzML	boolean; TRUE if mzML to be used FALSE if .csv file to be used
mzRback	character; backend to use for mzR parsing

Value

purityD object

Examples

```
datapth <- system.file("extdata", "dims", "mzML", package="msPurityData")
inDF <- Getfiles(datapth, pattern=".mzML", check = FALSE, cStrt = FALSE)
ppDIMS <- purityD(fileList=inDF, cores=1, mzML=TRUE)
```

---

iwNormGauss *Gaussian normalisation for isolation window efficiency*

Description

Creates a function based on a gaussian curve shape that will normalise any intensity values within a defined isolation window.

The function that is created will output a value between 0 to 1 based on the position between the minOff and maxOff params. (The value 1.0 being equivalent to 100

Usage

```
iwNormGauss(sdlim = 3, minOff = -0.5, maxOff = +0.5)
```

Arguments

sdlim	numerical; Standard deviation limit for gaussian curve
minOff	numerical; Offset to the 'left' for the precursor range. (Should be negative)
maxOff	character; Offset to the 'left' for the precursor range. (Should be positive)

Value

normalisation function for selected range.

Examples

```
iwNormFun <- iwNormGauss(minOff=-0.5, maxOff=0.5)
pm <- data.frame(mz=c(99.5, 99.9, 100, 100.1, 100.5),i=c(1000, 1000, 1000, 1000, 1000))
mzmax = 100.5
mzmin = 99.5
middle <- mzmax-(mzmax-mzmin)/2
adjustmz = pm$mz-middle

# normalise the intensities
pm$normi = pm$i*iwNormFun(adjustmz)
```

iwNormQE.5 *Q-Exactive +/- 0.5 range, normalisation for isolation window efficiency*

Description

Creates a function based on a previous experimental analysis of a Q-Exactive at +/- 0.5 isolation window efficiency. See http://pubs.acs.org/doi/abs/10.1021/acs.analchem.6b04358

The function that is created will output a value between 0 to 1 based on the position between the minOff and maxOff params

NOTE: The resulting function will work for values greater that 0.5 and less than -0.5.

This is because (on our instrument tested at least) when using a window of +/- 0.5, the isolation is NOT confined to the +/-0.5 Da window. Resulting in ions from outside the window being isolated. For this reason the function can normalise values outside of the the +/- 1 Da range. Please see above paper figure 3 for more details.

Usage

```
iwNormQE.5()
```

Value

normalisation function for +/- 0.5 range for Q-Exactive

Examples

```
iwNormFun <- iwNormQE.5()
pm <- data.frame(mz=c(99.5, 99.9, 100, 100.1, 100.5),i=c(1000, 1000, 1000, 1000, 1000))
mzmax = 100.5
mzmin = 99.5
middle <- mzmax-(mzmax-mzmin)/2
adjustmz = pm$mz-middle

# normalise the intensities
pm$normi = pm$i*iwNormFun(adjustmz)
```

iwNormRcosine *Raised cosine normalisation for isolation window efficiency*

Description

Creates a function based on a rasied cosine curve shape that will normalise any intensity values within a defined isolation window

The function that is created will output a value between 0 to 1 based on the position between the minOff and maxOff params

Usage

```
iwNormRcosine(minOff = -0.5, maxOff = +0.5)
```

Arguments

minOff	numerical; Offset to the 'left' for the precursor range. (Should be negative)
maxOff	character; Offset to the 'left' for the precursor range. (Should be positive)

Value

normalisation function for selected range

Examples

```
iwNormFun <- iwNormRcosine()
pm <- data.frame(mz=c(99.5, 99.9, 100, 100.1, 100.5),i=c(1000, 1000, 1000, 1000, 1000))
mzmax = 100.5
mzmin = 99.5
middle <- mzmax-(mzmax-mzmin)/2
adjustmz = pm$mz-middle

# normalise the intensities
pm$normi = pm$i*iwNormFun(adjustmz)
```

---

pcalc *Perform purity calculation on a peak matrix*

Description

This is the main purity calculation that is performed in purityX, purityD and purityA.

- Takes in a matrix of peaks
- gets isolation window based on mzmin mzmax
- locates the mz target in the peak matrix
- removes isotopic peaks
- removes any peaks below limit (percentage of target peak intensity)
- normalises
- Calculates purity: Divides the target peak intensity by the total peak intensity for the isolation window

Usage

```
pcalc(peaks, mzmin, mzmax, mztarget, ppm = NA, iwNorm = FALSE,
  iwNormFun = NULL, ilim = 0, targetMinMZ = NA, targetMaxMZ = NA,
  isotopes = FALSE, im = NULL)
```

Arguments

peaks	matrix; Matrix of peaks consisting of 2 columns: mz and i
mzmin	numeric; Isolation window (min)
mzmax	numeric; Isolation window (max)
mztarget	numeric; The mz window to target in the isolation window

ppm	numeric; PPM tolerance for the target mz value. If NA will presume targetMinMZ and targetMaxMZ will be used
iwNorm	boolean; If TRUE then the intensity of the isolation window will be normalised based on the iwNormFun function
iwNormFun	function; A function to normalise the isolation window intensity. The default function is very generalised and just accounts for edge effects
ilim	numeric; All peaks less than this percentage of the target peak will be removed from the purity calculation, default is 5% (0.05)
targetMinMZ	numeric; Range to look for the mztarget (min)
targetMaxMZ	numeric; Range to look for the mztarget (max)
isotopes	boolean; TRUE if isotopes are to be removed
im	matrix; Isotope matrix, default removes C13 isotopes (single, double and triple bonds)

Value

a vector of the purity score and the number of peaks in the window e.g c(purity, pknm)

Examples

```
pm <- rbind(c(100, 1000),c(101.003, 10))
pcalc(pm, mzmin = 98, mzmax = 102, mztarget=100, ppm=5)
pcalc(pm, mzmin = 98, mzmax = 102, mztarget=100, ppm=5, isotopes = TRUE)
```

---

purityA *Assess the purity of multiple LC-MS/MS or DI-MS/MS files (constructor)*

Description

Constructor for the purityA class.

Given a vector of LC-MS/MS or DI-MS/MS mzML file paths calculate the precursor purity of each MS/MS scan

Will automatically determine the isolation widths offsets from the mzML file. For some vendors though this is not recorded (Agilent). In these cases the offsets should be given as a parameter.

In the case of Agilent only the "narrow" isolation is supported. This roughly equates to +/- 0.65 Da (depending on the instrument). If the file is detected as originating from an Agilent instrument the isolation widths will automatically be set as +/- 0.65 Da.

Usage

```
purityA(fileList, cores = 1, mostIntense = FALSE, nearest = TRUE,
  offsets = NA, plotP = FALSE, plotdir = NULL, interpol = "linear",
  iwNorm = FALSE, iwNormFun = NULL, ilim = 0.05, mzRback = "pwiz",
  isotopes = TRUE, im = NULL)
```

Arguments

fileList	vector; mzML file paths for MS/MS spectra
cores	numeric; Number of cores to use
mostIntense	boolean; True if the most intense peak is used for calculation. False if the centered peak is used
nearest	boolean; True if the peak selected is from either the preceding scan or the nearest.
offsets	vector; Overide the isolation offsets found in the mzML filee.g. c(0.5, 0.5)
plotP	boolean; If TRUE a plot of the purity is to be saved
plotdir	vector; If plotP is TRUE plots will be saved to this directory
interpol	character; type of interolation to be performed "linear" or "spline" (Spline option is only included for testing purposes, linear should be used for all standard cases, isotope removal is also not available for the spline option)
iwNorm	boolean; If TRUE then the intensity of the isolation window will be normalised based on the iwNormFun function
iwNormFun	function; A function to normalise the isolation window intensity. The default function is very generalised and just accounts for edge effects
ilim	numeric; All peaks less than this percentage of the target peak will be removed from the purity calculation, default is 5% (0.05)
mzRback	character; backend to use for mzR parsing
isotopes	boolean; TRUE if isotopes are to be removed
im	matrix; Isotope matrix, default removes C13 isotopes (single, double and triple bonds)

Value

a dataframe of the purity score of the ms/ms spectra

See Also

assessPuritySingle

Examples

```
filepths <- system.file("extdata", "lcms", "mzML", "LCMSMS_1.mzML", package="msPurityData")
pa <- purityA(filepths)
```

---

purityD-class *An S4 class to represent a DI-MS purityD*

Description

The class used to assess anticipated purity from a DI-MS run

Arguments

.Object	object; purityD object
fileList	data.frame; Created using GetFiles, data.frame with filepaths and sample class information
cores	numeric; Number of cores used to perform Hierarchical clustering WARNING: memory intensive, default 1
mzML	boolean; TRUE if mzML to be used FALSE if .csv file to be used

Value

purityD object

Examples

```
datapth <- system.file("extdata", "dims", "mzML", package="msPurityData")
inDF <- Getfiles(datapth, pattern=".mzML", check = FALSE, cStrt = FALSE)
ppDIMS <- purityD(fileList=inDF, cores=1, mzML=TRUE)
```

---

purityX *Assessing anticipated purity of XCMS features from an LC-MS run*

Description

Constructor for the purityX class.

Given an XCMS object get the anticipated precursor purity of the grouped peaks

Usage

```
purityX(xset, purityType = "purityFWHMmedian", offsets = c(0.5, 0.5),
  fileignore = NULL, cores = 1, xgroups = NULL, iwNorm = FALSE,
  iwNormFun = NULL, ilim = 0.05, plotP = FALSE, mzRback = "pwiz",
  isotopes = FALSE, im = NULL, singleFile = 0, rtrawColumns = FALSE,
  saveEIC = FALSE, sqlitePth = NULL)
```

Arguments

xset	object; xcms object
purityType	character; Area and average used for the purity predictions. Options are "purityFWHMmedian", "purityFWmedian", "purityFWHMmean", "purityFWmean"
offsets	vector; vector of the isolation window upper and lower offsets
fileignore	vector; vector of files to ignore for the prediction calculation
cores	numeric; number of cores to use
xgroups	vector; vector of xcms groups to perform prediction on
iwNorm	boolean; if TRUE then the intensity of the isolation window will be normalised based on the iwNormFun function
iwNormFun	function; A function to normalise the isolation window intensity. The default function is very generalised and just accounts for edge effects

ilim	numeric; All peaks less than this percentage of the target peak will be removed from the purity calculation, default is 5% (0.05)
plotP	boolean; TRUE if plot of the EIC of feature and associated contamination is the be save to the working directory
mzRback	character; backend to use for mzR parsing
isotopes	boolean; TRUE if isotopes are to be removed
im	matrix; Isotope matrix, default removes C13 isotopes (single, double and triple bonds)
singleFile	numeric; If just a single file for purity is to be calculated (rather than the grouped XCMS peaks). Uses the index of the files in xcmsSet object. If zero this is ignored.
rtrawColumns	boolean; TRUE if the rt_raw values are included as additional columns in the @peaks slot (only required if using the obiwarp)
saveEIC	boolean; If True extracted ion chromatograms will be saved to SQLite database
sqlitePth	character; If saveEIC True, then a path to sqlite database can be used. If NULL then a database will be created in the working directory called eics

Value

a purityX object containing a dataframe of predicted purity scores

Examples

```
msPths <- list.files(system.file("extdata", "lcms", "mzML", package="msPurityData"), full.names = TRUE, patt
xset <- xcms::xcmsSet(msPths)
xset <- xcms::group(xset)
xset <- xcms::retcor(xset)
xset <- xcms::group(xset)
ppLCMS <- purityX(xset, cores = 1, xgroups = c(1, 2))
```

---

show,purityA-method *Show method for purityA class*

Description

print statement for purityA class

Usage

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

Arguments

object	object; purityA object

Value

a print statement of regarding object

show,purityD-method *Show method for purityD*

Description

Show method for purityD object

Usage

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

Arguments

object	= purityD object

Value

a print statement of regarding object

show,purityX-method *Show method for purityX*

Description

Show method for purityX object

Usage

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

Arguments

object	object; purityX object

Value

a print statement of regarding object

`spectral_matching` *Spectral matching*

Description

Perform spectral matching to spectral libraries using dot product cosine on a LC-MS/MS dataset and link to XCMS features.

Usage

```
spectral_matching(target_db_pth, ra_thres_l = 0, ra_thres_t = 2,
  cores = 1, pol = "positive", ppm_tol_prod = 10, ppm_tol_prec = 5,
  score_thres = 0.6, topn = NA, db_name = NA, library_db_pth = NA,
  instrument_types = NA, library_sources = "massbank", scan_ids = NA,
  pa = NA, xset = NA, grp_peaklist = NA, out_dir = ".")
```

Arguments

`target_db_pth`	character; Path of the database of targets that will be searched against the library spectra. Generated either from frag4feature or from create_database functions.
`ra_thres_l`	numeric; Relative abundance threshold for library spectra
`ra_thres_t`	numeric; Relative abundance threshold for target spectra (Peaks below this RA threshold will be excluded)
`cores`	numeric; Number of cores to use
`pol`	character; Polarity ['positive' or 'negative']
`ppm_tol_prod`	numeric; PPM tolerance to match to product
`ppm_tol_prec`	numeric; PPM tolerance to match to precursor
`score_thres`	numeric; Dot product cosine score threshold
`topn`	numeric [optional]; Only use top n matches
`db_name`	character [optional]; Name of the result database (e.g. can use CAMERA peaklist)
`library_db_pth`	character [optional]; path to library spectral SQLite database. Defaults to msPurityData package data.
`instrument_types`	vector [optional]; Vector of instrument types, defaults to all
`library_sources`	vector [optional]; Vector of library sources. Default option is for massbank only but the 'lipidblast' library is also available
`scan_ids`	vector [optional]; Vector of unique scan ids calculated from msPurity "pid". These scans will on used for the spectral matching. All scans will be used if set to NA
`pa`	purityA object [deprecated]; If target_db_pth set to NA, a new database can be created using pa, xset and grp_peaklist
`xset`	xcms object [deprecated]; If target_db_pth set to NA, a new database can be created using pa, xset and grp_peaklist
`grp_peaklist`	dataframe [deprecated]; If target_db_pth set to NA, a new database can be created using pa, xset and grp_peaklist
`out_dir`	character [deprecated]; If target_db_pth set to NA, Out directory for the SQLite result database

Value

list of database details and dataframe summarising the results for the xcms features

Examples

```
msmsPths <- list.files(system.file("extdata", "lcms", "mzML", package="msPurityData"), full.names = TRUE, pa
xset <- xcms::xcmsSet(msmsPths, nSlaves = 1)
xset <- xcms::group(xset)
xset <- xcms::retcor(xset)
xset <- xcms::group(xset)

pa  <- purityA(msmsPths)
pa <- frag4feature(pa, xset, create_db=TRUE)
#NOTE that scan_ids here are refer the unique scan id calculated by purityA (pids).
#Only required if you want to limit the spectral matching to certain scans
result <- spectral_matching(pa@db_path, scan_ids = c(1120,  366, 1190, 601,  404,1281, 1323, 1289))
```

---

subtract,purityD-method

Using Subtract MZ values based on ppm tolerance and noise ratio

---

Description

Uses a purityD object with references to multiple MS files. Subtract blank peaks from the sample peaks see subtractMZ for more information

Usage

```
## S4 method for signature 'purityD'
subtract(Object, byClass = TRUE, mapping = c("sample",
  "blank"), ppm = 5, s2bthres = 10)
```

Arguments

Object	object; purityD object
byClass	boolean; subtract within each class
mapping	parameter not functional (TODO)
ppm	numeric = ppm tolerance
s2bthres	numeric = threshold for the samp2blank (i1/i2)

Value

purityD object with averaged spectra

See Also

subtractMZ

Examples

```
datapth <- system.file("extdata", "dims", "mzML", package="msPurityData")
inDF <- Getfiles(datapth, pattern=".mzML", check = FALSE, cStrt = FALSE)

ppDIMS <- purityD(inDF, cores=1)
ppDIMS <- averageSpectra(ppDIMS)
ppDIMS <- filterp(ppDIMS, thr = 5000)
ppDIMS <- subtract(ppDIMS)
```

`subtractMZ` *Subtract MZ values based on ppm tolerance and noise ratio*

Description

This function is intended for blank subtraction of mz values from two peaklists. It takes in 2 vectors of mz values and 2 coresponding vectors of Intensity values.

The second mz values are subtracted from the first set within an MZ tolerance.

However, if the mz match but the intensity is above a defined threshold then they are not subtracted

Usage

```
subtractMZ(mz1, mz2, i1, i2, ppm = 5, s2bthres = 10)
```

Arguments

`mz1`	vector = mz values to start with
`mz2`	vector = mz values to subtract
`i1`	vector = i values for mz1
`i2`	vector = i values for mz2
`ppm`	numeric = ppm tolerance
`s2bthres`	numeric = threshold for the samp2blank (i1/i2)

Value

a vector of the remaining mz values

Examples

```
mz1 <- c(100.001, 200.002, 300.302)
mz2 <- c(100.004, 200.003, 500.101)
i1 <- c(100, 100, 100)
i2 <- c(100, 10000, 100)

subtractMZ(mz1, mz2, i1, i2, ppm=5, s2bthres =10)
```

validate,purityA-method

Validate precursor purity predictions using LC-MS and LC-MS/MS dataset

Description

The method is used to validate the precursor purity predictions made from an LC-MS dataset

Usage

```
## S4 method for signature 'purityA'
validate(pa, ppLCMS)
```

Arguments

pa	object; purityA object
ppLCMS	object; purityX object

Value

purityA object

writeOut,purityD-method

Using purityD object, save peaks as text files

Description

Uses a purityD object with references to multiple MS files. Predicts the purity of the processed sample files

Usage

```
## S4 method for signature 'purityD'
writeOut(Object, outDir, original)
```

Arguments

Object	object; purityD object
outDir	character; Directory to save text files
original	boolean; If the original (unprocessed) files are to be saved to text files

Value

purityD object

Index

assessPuritySingle, 2, *19*
averageSpectra
(averageSpectra,purityD-method), 3
averageSpectra,purityD-method, 3
averageSpectraSingle, *4*, 5

create_database, 6

dimsPredictPurity
(dimsPredictPurity,purityD-method), 7
dimsPredictPurity,purityD-method, 7
dimsPredictPuritySingle, *7*, 8

filterp (filterp,purityD-method), 9
filterp,purityD-method, 9
frag4feature
(frag4feature,purityA-method), 10
frag4feature,purityA-method, 10

get_additional_mzml_meta, 12
Getfiles, 11
getP (getP,purityD-method), 11
getP,purityD-method, 11
groupPeaks (groupPeaks,purityD-method), 13
groupPeaks,purityD-method, 13
groupPeaksEx, 13

initialize,purityD-method, 14
iwNormGauss, 15
iwNormQE.5, 16
iwNormRcosine, 16

pcalc, 17
purityA, *3*, 18
purityD (purityD-class), 19
purityD-class, 19
purityX, 20

show,purityA-method, 21
show,purityD-method, 22
show,purityX-method, 22

spectral_matching, 23
subtract (subtract,purityD-method), 24
subtract,purityD-method, 24
subtractMZ, *24*, 25

validate (validate,purityA-method), 26
validate,purityA-method, 26

writeOut (writeOut,purityD-method), 26
writeOut,purityD-method, 26