

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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URL <https://github.com/computational-metabolomics/msPurity/>

Description msPurity R package was developed to:

- 1) Assess the spectral quality of fragmentation spectra by evaluating the “precursor ion purity”.
- 2) Process fragmentation spectra.
- 3) Perform spectral matching.

What is precursor ion purity? -What we call “Precursor ion purity” is a measure of the contribution of a selected precursor peak in an isolation window used for fragmentation. The simple calculation involves dividing the intensity of the selected precursor peak by the total intensity of the isolation window. When assessing MS/MS spectra this calculation is done before and after the MS/MS scan of interest and the purity is interpolated at the recorded time of the MS/MS acquisition. Additionally, isotopic peaks can be removed, low abundance peaks are removed that are thought to have limited contribution to the resulting MS/MS spectra and the isolation efficiency of the mass spectrometer can be used to normalise the intensities used for the calculation.

Encoding UTF-8

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LazyData TRUE

BugReports <https://github.com/computational-metabolomics/msPurity/issues/new>

Depends Rcpp

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 'iw-norm.R' 'matching-algs.R' 'meta_extract.R' 'msPurity.R'
 'pcalc.R' 'purityA-0-class.R' 'purityA-av-spectra.R'
 'purityA-constructor.R' 'purityA-create-msp.R'
 'purityA-filter-frag-spectra.R' 'purityA-frag4feature.R'
 'purityA-validate.R' 'purityD-class.R' 'purityD-constructor.R'
 'purityD-av-spectra.R' 'purityD-dims-purity.R'
 'purityD-fileList.R' 'purityD-filterp.R' 'purityD-subtract.R'
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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 outputted 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,
    ppmInterp = 7
  )

```

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; Override the isolation offsets found in the mzML file.e.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) |
| ppmInterp | numeric; Set the ppm tolerance for the precursor ion purity interpolation. i.e. the ppm tolerance between the precursor ion found in the neighbouring scans. |

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)

```

averageAllFragSpectra,purityA-method

Using a purityA object, average and filter MS/MS spectra for each XCMS feature within and across MS data files (ignoring intra and inter relationships)

Description

General

Average and filter fragmentation spectra for each XCMS feature within and across MS data files (ignoring intra and inter relationships).

The averaging is performed using hierarchical clustering of the m/z values of each peaks, where m/z values within a set ppm tolerance will be clustered. The clustered peaks are then averaged (or summed).

The fragmentation can be filtered on the averaged spectra (with the arguments snr, rsd, minfrac, ra)

Example LC-MS/MS processing workflow

- Purity assessments
 - (mzML files) -> purityA -> (pa)
- XCMS processing
 - (mzML files) -> xcms.findChromPeaks -> (optionally) xcms.adjustRtime -> xcms.groupChromPeaks -> (xcmsObj)
 - — *Older versions of XCMS* — (mzML files) -> xcms.xcmsSet -> xcms.group -> xcms.retcor -> xcms.group -> (xcmsObj)
- Fragmentation processing
 - (xcmsObj, pa) -> frag4feature -> filterFragSpectra -> **averageAllFragSpectra** -> create-Database -> spectralMatching -> (sqlite spectral database)

Usage

```
## S4 method for signature 'purityA'
averageAllFragSpectra(
  pa,
  minfrac = 0.5,
  minnum = 1,
  ppm = 5,
  snr = 0,
  ra = 0,
  av = "median",
  sumi = TRUE,
  rmp = FALSE,
  cores = 1
)
```

Arguments

| | |
|---------|--|
| pa | object; purityA object |
| minfrac | numeric; minimum ratio of the peak fraction (peak count / total peaks) across all (ignoring intra and inter relationships) |
| minnum | numeric; minimum number of times peak is present across all fragmentation spectra (ignoring intra and inter relationships) |
| ppm | numeric; ppm threshold to average across all scans (ignoring intra and inter relationships) |
| snr | numeric; minimum signal-to-noise of the peak across all (ignoring intra and inter relationships) |
| ra | numeric; minimum relative abundance of the peak fraction across all (ignoring intra and inter relationships) |
| av | character; type of averaging to use (median or mean) |
| sumi | boolean; TRUE if the intensity for each peak is summed across averaged spectra |
| rmp | boolean; TRUE if peaks are to be removed that do not meet the threshold criteria. Otherwise they will just be flagged |
| cores | numeric; Number of cores for multiprocessing |

Value

Returns a purityA object (pa) with the following slots now with data

- pa@av_spectra: the average spectra is recorded here stored as a list. E.g. pa@av_spectra\$1\$av_all would give the average spectra for grouped feature 1.
- pa@av_all_params: The parameters used are recorded here

Each spectra in the av_spectra list contains the following columns:

- cl: id of clustered (averaged) peak
- mz: average m/z
- i: average intensity
- snr: average signal to noise ratio
- rsd: relative standard deviation
- count: number of clustered peaks
- total: total number of potential scans to be used for averaging
- inPurity: average precursor ion purity
- ra: average relative abundance
- frac: the fraction of clustered peaks (e.g. the count/total)
- snr_pass_flag: TRUE if snr threshold criteria met
- minfrac_pass_flag: TRUE if minfrac threshold criteria
- ra_pass_flag: TRUE if ra threshold criteria met
- pass_flag: TRUE if all threshold criteria met

Examples

```

##### XCMS #####
## Read in MS data
#msmsPths <- list.files(system.file("extdata", "lcms", "mzML",
#                               package="msPurityData"), full.names = TRUE, pattern = "MSMS")
#ms_data = readMSData(msmsPths, mode = 'onDisk', msLevel. = 1)

## Find peaks in each file
#cwp <- CentWaveParam(snthresh = 5, noise = 100, ppm = 10, peakwidth = c(3, 30))
#xcmsObj <- xcms::findChromPeaks(ms_data, param = cwp)

## Optionally adjust retention time
#xcmsObj <- adjustRtime(xcmsObj , param = ObiwrapParam(binSize = 0.6))

## Group features across samples
#pdp <- PeakDensityParam(sampleGroups = c(1, 1), minFraction = 0, bw = 30)
#xcmsObj <- groupChromPeaks(xcmsObj , param = pdp)

##### msPurity #####
#pa <- purityA(msmsPths)
#pa <- frag4feature(pa, xcmsObj)
#pa <- filterFragSpectra(pa)
#pa <- averageAllFragSpectra(pa)

## Run from previously generated data
pa <- readRDS(system.file("extdata", "tests", "purityA",
                        "3_filterFragSpectra_pa.rds", package="msPurity"))
pa <- averageAllFragSpectra(pa)

```

averageInterFragSpectra,purityA-method

Using a purityA object, average and filter fragmentation spectra for each XCMS feature across multiple MS data files

Description**General**

Average and filter fragmentation spectra for each XCMS feature across MS data files. This can only be run after averageIntraFragSpectra has been used.

The averaging is performed using hierarchical clustering of the m/z values of each peaks, where m/z values within a set ppm tolerance will be clustered. The clustered peaks are then averaged (or summed).

The fragmentation can be filtered on the averaged spectra (with the arguments snr, rsd, minfrac and ra)

Example LC-MS/MS processing workflow

- Purity assessments
 - (mzML files) -> purityA -> (pa)
- XCMS processing
 - (mzML files) -> xcms.findChromPeaks -> (optionally) xcms.adjustRtime -> xcms.groupChromPeaks -> (xcmsObj)
 - — *Older versions of XCMS* — (mzML files) -> xcms.xcmsSet -> xcms.group -> xcms.retcor -> xcms.group -> (xcmsObj)
- Fragmentation processing
 - (xcmsObj, pa) -> frag4feature -> filterFragSpectra -> averageIntraFragSpectra -> **averageInterFragSpectra** -> createDatabase -> spectralMatching -> (sqlite spectral database)

Usage

```
## S4 method for signature 'purityA'
averageInterFragSpectra(
  pa,
  minfrac = 0.5,
  minnum = 1,
  ppm = 5,
  snr = 0,
  ra = 0,
  av = "median",
  sumi = TRUE,
  rmp = FALSE,
  cores = 1
)
```

Arguments

| | |
|---------|---|
| pa | object; purityA object |
| minfrac | numeric; minimum ratio of the peak fraction (peak count / total peaks) across files |
| minnum | numeric; minimum number of times peak is present across fragmentation spectra across files |
| ppm | numeric; ppm threshold to average across files |
| snr | numeric; minimum signal-to-noise of the peak across files |
| ra | numeric; minimum relative abundance of the peak across files |
| av | character; type of averaging to use (median or mean) |
| sumi | boolean; TRUE if the intensity for each peak is summed across averaged spectra |
| rmp | boolean; TRUE if peaks are to be removed that do not meet the threshold criteria. Otherwise they will just be flagged |
| cores | numeric; Number of cores for multiprocessing |

Value

Returns a purityA object (pa) with the following slots now with data

- pa@av_spectra: the average spectra is recorded here stored as a list. e.g. "pa@av_spectra\$1\$av_inter" would give the average spectra for grouped feature 1
- pa@av_intra_params: The parameters used are recorded here

Each spectra in the av_spectra list contains the following columns: *

- cl: id of clustered (averaged) peak
- mz: average m/z
- i: average intensity
- snr: average signal to noise ratio
- rsd: relative standard deviation
- count: number of clustered peaks
- total: total number of potential scans to be used for averaging
- inPurity: average precursor ion purity
- ra: average relative abundance
- frac: the fraction of clustered peaks (e.g. the count/total)
- snr_pass_flag: TRUE if snr threshold criteria met
- minfrac_pass_flag: TRUE if minfrac threshold criteria
- ra_pass_flag: TRUE if ra threshold criteria met
- pass_flag: TRUE if all threshold criteria met

Examples

```
#===== XCMS =====
## Read in MS data
#msmsPths <- list.files(system.file("extdata", "lcms", "mzML",
#                               package="msPurityData"), full.names = TRUE, pattern = "MSMS")
#ms_data = readMSData(msmsPths, mode = 'onDisk', msLevel. = 1)

## Find peaks in each file
#cwp <- CentWaveParam(snthresh = 5, noise = 100, ppm = 10, peakwidth = c(3, 30))
#xcmsObj <- xcms::findChromPeaks(ms_data, param = cwp)

## Optionally adjust retention time
#xcmsObj <- adjustRtime(xcmsObj , param = ObiwrapParam(binSize = 0.6))

## Group features across samples
#pdp <- PeakDensityParam(sampleGroups = c(1, 1), minFraction = 0, bw = 30)
#xcmsObj <- groupChromPeaks(xcmsObj , param = pdp)

#===== msPurity =====
#pa <- purityA(msmsPths)
#pa <- frag4feature(pa, xcmsObj)
#pa <- averageIntraFragSpectra(pa)
```

```
#pa <- averageInterFragSpectra(pa)

## Run from previously generated data
pa <- readRDS(system.file("extdata", "tests", "purityA",
                          "4_averageIntraFragSpectra_no_filter_pa.rds",
                          package="msPurity"))
pa <- averageInterFragSpectra(pa)
```

averageIntraFragSpectra,purityA-method

Using a purityA object, average and filter fragmentation spectra for each XCMS feature within a MS data file

Description

General

Average and filter fragmentation spectra for each XCMS feature within a MS data file.

The averaging is performed using hierarchical clustering of the m/z values of each peaks, where m/z values within a set ppm tolerance will be clustered. The clustered peaks are then averaged (or summed).

The fragmentation can be filtered on the averaged spectra (with the arguments snr, rsd, minfrac and ra)

Example LC-MS/MS processing workflow

- Purity assessments
 - (mzML files) -> purityA -> (pa)
- XCMS processing
 - (mzML files) -> xcms.xcmsSet -> xcms.merge -> xcms.group -> xcms.retcor -> xcms.group -> (xcmsObj)
- XCMS processing (version >= 3)
 - (mzML files) -> MSnBase.readMSdata -> xcms.findChromPeaks -> xcms.groupChromPeaks -> xcms.adjustRtime -> xcms.groupChromPeaks -> (xcmsObj)
- Fragmentation processing
 - (xcmsObj, pa) -> frag4feature -> filterFragSpectra -> **averageIntraFragSpectra** -> averageIntraFragSpectra -> createDatabase -> spectralMatching -> (sqlite spectral database)

Usage

```
## S4 method for signature 'purityA'
averageIntraFragSpectra(
  pa,
  minfrac = 0.5,
  minnum = 1,
  ppm = 5,
```

```

    snr = 0,
    ra = 0,
    av = "median",
    sumi = TRUE,
    rmp = FALSE,
    cores = 1
)

```

Arguments

| | |
|---------|---|
| pa | object; purityA object |
| minfrac | numeric; minimum ratio of the peak fraction (peak count / total peaks) within each file |
| minnum | numeric; minimum number of times peak is present across fragmentation spectra within each file |
| ppm | numeric; ppm threshold to average within each file |
| snr | numeric; minimum signal-to-noise of the peak within each file |
| ra | numeric; minimum relative abundance of the peak within each file |
| av | character; type of averaging to use (median or mean) |
| sumi | boolean; TRUE if the intensity for each peak is summed across averaged spectra |
| rmp | boolean; TRUE if peaks are to be removed that do not meet the threshold criteria. Otherwise they will just be flagged |
| cores | numeric; Number of cores for multiprocessing |

Value

Returns a purityA object (pa) with the following slots now with data

- pa@av_spectra: the average spectra is recorded here stored as a list. e.g. "pa@av_spectra\$1\$av_intra\$1" would give the average spectra for grouped feature 1 and for file 1.
- pa@av_intra_params: The parameters used are recorded here

Each spectra in the av_spectra list contains the following columns:

- cl: id of clustered (averaged) peak
- mz: average m/z
- i: average intensity
- snr: average signal to noise ratio
- rsd: relative standard deviation
- count: number of clustered peaks
- total: total number of potential scans to be used for averaging
- inPurity: average precursor ion purity
- ra: average relative abundance
- frac: the fraction of clustered peaks (e.g. the count/total)

- snr_pass_flag: TRUE if snr threshold criteria met
- minfrac_pass_flag: TRUE if minfrac threshold criteria
- ra_pass_flag: TRUE if ra threshold criteria met
- pass_flag: TRUE if all threshold criteria met

Examples

```

#===== XCMS =====
## Read in MS data
#msmsPths <- list.files(system.file("extdata", "lcms", "mzML",
#                               package="msPurityData"), full.names = TRUE, pattern = "MSMS")
#ms_data = readMSData(msmsPths, mode = 'onDisk', msLevel. = 1)

## Find peaks in each file
#cwpc <- CentWaveParam(snrthresh = 5, noise = 100, ppm = 10, peakwidth = c(3, 30))
#xcmsObj <- xcms::findChromPeaks(ms_data, param = cwpc)

## Optionally adjust retention time
#xcmsObj <- adjustRtime(xcmsObj , param = ObiwrapParam(binSize = 0.6))

## Group features across samples
#pdp <- PeakDensityParam(sampleGroups = c(1, 1), minFraction = 0, bw = 30)
#xcmsObj <- groupChromPeaks(xcmsObj , param = pdp)

#===== msPurity =====
#pa <- purityA(msmsPths)
#pa <- frag4feature(pa, xcmsObj)
#pa <- averageIntraFragSpectra(pa)

# Run from previously generated data (where class is 'XCMSnExp'):
pa <- readRDS(system.file("extdata", "tests", "purityA",
                        "2_frag4feature_pa.rds", package="msPurity"))
pa <- averageIntraFragSpectra(pa)

```

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, background, 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; Deprecated. 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)
```

combineAnnotations *Combine Annotations*

Description

Combine the annotation results from msPurity spectral matching, MetFrag, Sirius CSI:FingerID, probmetab and any generic MS1 lookup software (e.g. results from the BEAMS software)

The annotation results are then aligned by inchikey and XCMS grouped feature.

The tool has to be run with a local compound database (available on request - contact t.n.lawson@bham.ac.uk)

Usage

```
combineAnnotations(  
  sm_resultPth,  
  compoundDbPth,  
  metfrag_resultPth = NA,  
  sirius_csi_resultPth = NA,  
  probmetab_resultPth = NA,  
  ms1_lookup_resultPth = NA,  
  ms1_lookup_dbSource = "hmdb",  
  ms1_lookup_checkAdducts = FALSE,  
  ms1_lookup_keepAdducts = c("[M+H]+", "[M-H]-"),  
  weights = list(sm = 0.3, metfrag = 0.2, sirius_csifingerid = 0.2, probmetab = 0,  
    ms1_lookup = 0.05, biosim = 0.25),  
  compoundDbType = "sqlite",  
  compoundDbName = NA,  
  compoundDbHost = NA,  
  compoundDbPort = NA,  
  compoundDbUser = NA,  
  compoundDbPass = NA,  
  outPth = NA,  
  summaryOutput = TRUE  
)
```

Arguments

| | |
|----------------------|--|
| sm_resultPth | character; Path to the msPurity SQLite database used for spectral matching |
| compoundDbPth | character; Path to local compound database with pubchem, hmdb, KEGG and metab_compound summary table (full database available on request - contact t.n.lawson@bham.ac.uk). This is only applicable if using "compoundDbType sqlite") |
| metfrag_resultPth | character; Path to the tsv table of metfrag results |
| sirius_csi_resultPth | character; Path to the tsv table of Sirius CSI:Finger ID results |

createDatabase *Create database*

Description

General

Create an SQLite database of an LC-MS(/MS) experiment (replaces the create_database function).

Schema details can be found [here](#).

Example LC-MS/MS processing workflow

- Purity assessments
 - (mzML files) -> purityA -> (pa)
- XCMS processing
 - (mzML files) -> xcms.findChromPeaks -> (optionally) xcms.adjustRtime -> xcms.groupChromPeaks -> (xcmsObj)
 - — *Older versions of XCMS* — (mzML files) -> xcms.xcmsSet -> xcms.group -> xcms.retcor -> xcms.group -> (xcmsObj)
- Fragmentation processing
 - (xcmsObj, pa) -> frag4feature -> filterFragSpectra -> averageAllFragSpectra -> **create-Database** -> spectralMatching -> (sqlite spectral database)

Usage

```
createDatabase(
  pa,
  xcmsObj,
  xsa = NULL,
  outDir = ".",
  grpPeaklist = NA,
  dbName = NA,
  metadata = NA,
  xset = NA
)
```

Arguments

| | |
|---------|--|
| pa | purityA object; Needs to be the same used for frag4feature function |
| xcmsObj | xcms object of class XCMSnExp or xcmsSet; 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 |

| | |
|-------------|---|
| outDir | character; Out directory for the SQLite result database |
| grpPeaklist | dataframe (optional); Can use any peak dataframe. Still needs to be derived from the xset object though |
| dbName | character (optional); Name of the result database |
| metadata | list; A list of metadata to add to the s_peak_meta table |
| xset | xcms object of class XCMSnExp or xcmsSet; (Deprecated - if provided, will replace variable 'obj') |

Value

path to SQLite database and database name

Examples

```

library(xcms)
library(MSNbase)
library(magrittr)
##### XCMS #####
## Read in MS data
msmsPths <- list.files(system.file("extdata", "lcms", "mzML",
                                package="msPurityData"), full.names = TRUE, pattern = "MSMS")
ms_data = readMSData(msmsPths, mode = 'onDisk', msLevel. = 1)

## Find peaks in each file
cwp <- CentWaveParam(snthresh = 5, noise = 100, ppm = 10, peakwidth = c(3, 30))
xcmsObj <- xcms::findChromPeaks(ms_data, param = cwp)

## Optionally adjust retention time
xcmsObj <- adjustRtime(xcmsObj, param = ObiwrapParam(binSize = 0.6))

## Group features across samples
pdp <- PeakDensityParam(sampleGroups = c(1, 1), minFraction = 0, bw = 30)
xcmsObj <- groupChromPeaks(xcmsObj, param = pdp)

##### msPurity #####
pa <- purityA(msmsPths)
pa <- frag4feature(pa = pa, xcmsObj = xcmsObj)
pa <- filterFragSpectra(pa, allfrag=TRUE)
pa <- averageAllFragSpectra(pa)
dbPth <- createDatabase(pa, xcmsObj, metadata=list('polarity'='positive', 'instrument'='Q-Exactive'))

td <- tempdir()
db_pth = createDatabase(pa = pa, xcmsObj = xcmsObj, outDir = td)

```

```
createMSP,purityA-method
```

Using a purityA object, create an MSP file of fragmentation spectra

Description

General

Create an MSP file for all the fragmentation spectra that has been linked to an XCMS feature via frag4feature. Can export all the associated scans individually or the averaged fragmentation spectra can be exported.

Additional metadata can be included in a dataframe (each column will be added to metadata of the MSP spectra). The dataframe must contain the column "grpId" corresponding to the XCMS grouped feature.

Example LC-MS/MS processing workflow

- Purity assessments
 - (mzML files) -> **purityA** -> (pa)
- XCMS processing
 - (mzML files) -> xcms.findChromPeaks -> (optionally) xcms.adjustRtime -> xcms.groupChromPeaks -> (xcmsObj)
 - — *Older versions of XCMS* — (mzML files) -> xcms.xcmsSet -> xcms.group -> xcms.retcor -> xcms.group -> (xcmsObj)
- Fragmentation processing
 - (xcmsObj, pa) -> frag4feature -> filterFragSpectra -> averageIntraFragSpectra -> averageIntraFragSpectra -> **createMSP** -> (MSP file)

Usage

```
## S4 method for signature 'purityA'
createMSP(
  pa,
  msp_file_pth = NULL,
  metadata = NULL,
  metadata_cols = NULL,
  xcms_groupids = NULL,
  method = "all",
  adduct_split = TRUE,
  filter = TRUE,
  msp_schema = "massbank",
  intensity_ra = "intensity_ra",
  include_adducts = ""
)
```

Arguments

| | |
|-----------------|--|
| pa | object; purityA object |
| msp_file_pth | character; Name of the output msp file, if NULL the file "frag_spectra_time stamp.msp" will be created in the current directory |
| metadata | data.frame; Data frame with additional compound information to include in msp output |
| metadata_cols | vector; Column names of meta data to incorporate into name |
| xcms_groupids | vector; XCMS group id's to extract ms/ms data for |
| method | character; "all" will export all matching ms/ms spectra to xcms features, "max" will use spectra with the highest intensity, "av_intra" will use the intra file averaged spectra (within file), "av_inter" will use the inter file (across file) averaged spectra, "av_all" will use the averaged spectra (ignoring inter and intra) |
| adduct_split | boolean; If either "adduct" or MS\$FOCUSED_ION: PRECURSOR_TYPE column is in metadata then each adduct will have it's own MSP spectra. (Useful, if the MSP file will be used for further annotation) |
| filter | boolean; TRUE if filtered peaks are to be removed |
| msp_schema | character; Either MassBank (Europe) or MoNA style of MSP file format to be used ('massbank' or 'mona') |
| intensity_ra | character; Either 'intensity', 'ra' (relative abundance) or 'intensity_ra' (intensity and relative abundance) to be written to the MSP file |
| include_adducts | character; Additional adducts to include as a string separated by white a space (e.g. [M+H]+ [M+Na]+) |

Value

Returns a MSP file with the selected spectra and metadata

Examples

```
##### XCMS #####
## Read in MS data
#msmsPths <- list.files(system.file("extdata", "lcms", "mzML",
#                               package="msPurityData"), full.names = TRUE, pattern = "MSMS")
#ms_data = readMSData(msmsPths, mode = 'onDisk', msLevel. = 1)

## Find peaks in each file
#cwp <- CentWaveParam(snthresh = 5, noise = 100, ppm = 10, peakwidth = c(3, 30))
#xcmsObj <- xcms::findChromPeaks(ms_data, param = cwp)

## Optionally adjust retention time
#xcmsObj <- adjustRtime(xcmsObj, param = ObiwrapParam(binSize = 0.6))

## Group features across samples
#pdp <- PeakDensityParam(sampleGroups = c(1, 1), minFraction = 0, bw = 30)
#xcmsObj <- groupChromPeaks(xcmsObj, param = pdp)
```

```

##### msPurity #####
#pa <- purityA(msmsPths)
#pa <- frag4feature(pa = pa, xcmsObj = xcmsObj)
#pa <- filterFragSpectra(pa, allfrag=TRUE)
#pa <- averageAllFragSpectra(pa)
#createMSP(pa)

pa <- readRDS(system.file("extdata", "tests", "purityA",
                          "9_averageAllFragSpectra_with_filter_pa.rds",
                          package="msPurity"))

createMSP(pa)

```

create_database *Create database [deprecated](#)*

Description

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

msPurity::create_database is deprecated. Please use msPurity::createDatabase for future use

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

Examples

```
#msmsPths <- list.files(system.file("extdata", "lcms", "mzML",
#                             package="msPurityData"), full.names = TRUE, pattern = "MSMS")
#xset <- xcms::xcmsSet(msmsPths)
#xset <- xcms::group(xset)

#pa <- purityA(msmsPths)
#pa <- frag4feature(pa, xset)
#pa <- averageAllFragSpectra(pa)
#db_pth <- create_database(pa, xset)

# Run from previously generated data
pa <- readRDS(system.file("extdata", "tests", "purityA",
                        "9_averageAllFragSpectra_with_filter_pa_OLD.rds",
                        package="msPurity"))
xset <- readRDS(system.file("extdata", "tests", "xcms",
                          "msms_only_xset_OLD.rds", package="msPurity"))

# Need to ensure the filelists are matching
msmsPths <- list.files(system.file("extdata", "lcms", "mzML",
                                package="msPurityData"),
                      full.names = TRUE, pattern = "MSMS")
pa@fileList[1] <- msmsPths[basename(msmsPths)=="LCMSMS_1.mzML"]
pa@fileList[2] <- msmsPths[basename(msmsPths)=="LCMSMS_2.mzML"]
xset@filepaths[1] <- msmsPths[basename(msmsPths)=="LCMSMS_1.mzML"]
xset@filepaths[2] <- msmsPths[basename(msmsPths)=="LCMSMS_2.mzML"]
db_pth <- create_database(pa, xset)
```

dimsPredictPurity,purityD-method

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

Description

Assess the precursor purity of anticipated 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 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

| | |
|------------------------|--|
| <code>mztargets</code> | vector = mz targets to get predicted purity for |
| <code>filepth</code> | character = mzML file path or .csv file path |
| <code>minOffset</code> | numeric = isolation window minimum offset |
| <code>maxOffset</code> | numeric = isolation window maximum offset |
| <code>ppm</code> | numeric = tolerance for target mz value in each scan |
| <code>mzML</code> | boolean = Whether an mzML file is to be used or .csv file (TRUE == mzML) |
| <code>iwNorm</code> | boolean = if TRUE then the intensity of the isolation window will be normalised based on the iwNormFun function |
| <code>iwNormFun</code> | function = A function to normalise the isolation window intensity. The default function is very generalised and just accounts for edge effects |
| <code>ilim</code> | numeric = All peaks less than this percentage of the target peak will be removed from the purity calculation, default is 5% (0.05) |
| <code>mzRback</code> | 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, ppm=5, mzML=TRUE)
```

filterFragSpectra,purityA-method

Filter fragmentation spectra associated with an XCMS feature

Description**General**

Flag and filter features based on signal-to-noise ratio, relative abundance, intensity threshold and purity of the precursor ion.

Example LC-MS/MS processing workflow

- Purity assessments
 - (mzML files) -> purityA -> (pa)
- XCMS processing
 - (mzML files) -> xcms.findChromPeaks -> (optionally) xcms.adjustRtime -> xcms.groupChromPeaks -> (xcmsObj)
 - — *Older versions of XCMS* — (mzML files) -> xcms.xcmsSet -> xcms.group -> xcms.retcor -> xcms.group -> (xcmsObj)
- Fragmentation processing
 - (xcmsObj, pa) -> frag4feature -> **filterFragSpectra** -> averageAllFragSpectra -> create-Database -> spectralMatching -> (sqlite spectral database)

Usage

```
## S4 method for signature 'purityA'
filterFragSpectra(
  pa,
  ilim = 0,
  plim = 0.8,
  ra = 0,
  snr = 3,
  rmp = FALSE,
  snmeth = "median",
  allfrag = FALSE
)
```

Arguments

| | |
|---------|--|
| pa | object; purityA object |
| ilim | numeric; min intensity of a peak |
| plim | numeric; min precursor ion purity of the associated precursor for fragmentation spectra scan |
| ra | numeric; minimum relative abundance of a peak |
| snr | numeric; minimum signal-to-noise of a peak within each file |
| rmp | boolean; TRUE if peaks are to be removed that do not meet the threshold criteria. Otherwise they will just be flagged. |
| snmeth | character; Method to calculate signal to noise ration (either median or mean) |
| allfrag | boolean; Whether to filter on all fragmentation spectra or just the fragmentation spectra grouped to XCMS feature |

Value

Returns a purityA object with the pa@grpед_msms spectra matrices are updated with the following columns

- snr: Signal to noise ratio (calculated at scan level)
- ra: Relative abundance (calculated at scan level)
- purity_pass_flag: Precursor ion purity flag (1 pass, 0 fail)
- intensity_pass_flag: Intensity flag (1 pass, 0 fail)
- snr_pass_flag: Signal-to-noise pass flag (1 pass, 0 fail)
- ra_pass_flag: Relative abundance pass flag (1 pass, 0 fail)
- pass_flag: Overall pass flag, all flags must pass for this to pass (1 pass, 0 fail)

Examples

```
#===== XCMS =====
## Read in MS data
#msmsPths <- list.files(system.file("extdata", "lcms", "mzML"),
```

```

#           package="msPurityData"), full.names = TRUE, pattern = "MSMS")
#ms_data = readMSData(msmsPths, mode = 'onDisk', msLevel. = 1)

## Find peaks in each file
#cwp <- CentWaveParam(snthresh = 5, noise = 100, ppm = 10, peakwidth = c(3, 30))
#xcmsObj <- xcms::findChromPeaks(ms_data, param = cwp)

## Optionally adjust retention time
#xcmsObj <- adjustRtime(xcmsObj , param = ObiwrapParam(binSize = 0.6))

## Group features across samples
#pdp <- PeakDensityParam(sampleGroups = c(1, 1), minFraction = 0, bw = 30)
#xcmsObj <- groupChromPeaks(xcmsObj , param = pdp)

#==== msPurity =====
#pa <- purityA(msmsPths)
#pa <- frag4feature(pa, xcmsObj)
#pa <- filterFragSpectra(pa)

## Run from previously generated data
pa <- readRDS(system.file("extdata", "tests", "purityA",
                          "2_frag4feature_pa.rds", package="msPurity"))
pa <- filterFragSpectra(pa)

```

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)
```

flag_remove

Flag and remove unwanted peaks

Description

Filter, flag and remove unwanted peaks from xcms object (xcmsObj) of class XCMSnExp, xcmsSet or xsAnnotate. When the peaks are removed, the xcmsObj object can be regrouped (originally using xcms::group, now using xcms::groupChromPeaks). The function then checks if any blank peaks are still present and the process is repeated.

The output is a list object containing: 1) the updated xcms object, 2) the grouped peaklist and 3) the blank removed peaks

Usage

```
flag_remove(  
  xcmsObj,  
  pol = NA,  
  rsd_i_blank = NA,  
  minfrac_blank = 0.5,  
  rsd_rt_blank = NA,  
  ithres_blank = NA,  
  s2b = 10,  
  ref.class = "blank",  
  egauss_thr = NA,  
  rsd_i_sample = NA,  
  minfrac_sample = 0.7,  
  rsd_rt_sample = NA,  
  ithres_sample = NA,  
  minfrac_xcms = 0.7,  
  mzwid = 0.017,  
  bw = 5,  
  out_dir = ".",  
  temp_save = FALSE,  
  remove_spectra_bool = TRUE,  
  grp_rm_ids = NA,  
  xset = NA  
)
```

Arguments

| | |
|----------------------------------|--|
| <code>xcmsObj</code> | object; XCMSnExp, xcmsSet or xsAnnotate object |
| <code>pol</code> | str; polarity (just used for naming purpose for files being saved) [positive, negative, NA] |
| <code>rsd_i_blank</code> | numeric; RSD threshold for the blank |
| <code>minfrac_blank</code> | numeric; minimum fraction of files for features needed for the blank |
| <code>rsd_rt_blank</code> | numeric; RSD threshold for the RT of the blank |
| <code>ithres_blank</code> | numeric; Intensity threshold for the blank |
| <code>s2b</code> | numeric; fold change (sample/blank) needed for sample peak to be allowed. e.g. if s2b set to 10 and the recorded sample 'intensity' value was 100 and blank = 10. $1000/10 = 100$ so sample has fold change higher than the threshold and the peak is not considered a blank |
| <code>ref.class</code> | str; A string representing the class that will be used for the blank. |
| <code>egauss_thr</code> | numeric; Threshold for filtering out non gaussian shaped peaks. Note this only works if the verbose option was set for XCMS; |
| <code>rsd_i_sample</code> | numeric; RSD threshold for the sample |
| <code>minfrac_sample</code> | numeric; minimum fraction of files for features needed for the sample |
| <code>rsd_rt_sample</code> | numeric; RSD threshold for the RT of the sample |
| <code>ithres_sample</code> | numeric; Intensity threshold for the sample |
| <code>minfrac_xcms</code> | numeric; minfrac for xcms grouping |
| <code>mzwid</code> | numeric; xcms grouping parameter (corresponds to variable 'binSize' in XCMS3) |
| <code>bw</code> | numeric; xcms grouping parameter |
| <code>out_dir</code> | str; out directory |
| <code>temp_save</code> | boolean; Assign True if files for each step saved (for testing purposes) |
| <code>remove_spectra_bool</code> | bool; TRUE if flagged spectra is to be removed |
| <code>grp_rm_ids</code> | vector; vector of grouped_xcms peaks to remove (corresponds to the row from xcms::group output) |
| <code>xset</code> | object, DEPRECATED; xcmsSet object |

Value

list(xset, grp_peaklist, removed_peaks)

Examples

```
library(xcms)
library(MSnbase)
library(magrittr)
#read in files and data
msPths <-list.files(system.file("extdata", "lcms", "mzML", package="msPurityData"), full.names = TRUE)
ms_data = readMSData(msPths, mode = 'onDisk', msLevel. = 1)
```

```

#subset the data to focus on retention times 30-90 seconds and m/z values between 100 and 200 m/z.
rtr = c(30, 90)
mzr = c(100, 200)
ms_data = ms_data %>% filterRt(rt = rtr) %>% filterMz(mz = mzr)

##### perform feature detection in individual files
cwp <- CentWaveParam(snthresh = 3, noise = 100, ppm = 10, peakwidth = c(3, 30))
xcmsObj <- findChromPeaks(ms_data, param = cwp)
xcmsObj@phenoData@data$class = c('blank', 'blank', 'sample', 'sample')
xcmsObj@phenoData@varMetadata = data.frame('labelDescription' = 'sampleNames', 'class')
pdp <- PeakDensityParam(sampleGroups = xcmsObj@phenoData@data$class, minFraction = 0, bw = 5, binSize = 0.017)
xcmsObj <- groupChromPeaks(xcmsObj, param = pdp)

#### flag, filter and remove peaks, returning an updated xcmsObj (XCMSnExp or xcmsSet class), grouped_peaklist (data)
fr <- flag_remove(xcmsObj)

##### load from existing data
xcmsObj = readRDS(system.file("extdata", "tests", "purityA", "10_input_filterflagremove.rds", package="msPurity")

```

```
frag4feature.purityA-method
```

Using a purityA object, link MS/MS data to XCMS features

Description

General:

Assign fragmentation spectra (MS/MS) stored within a purityA class object to grouped features within an XCMS xset object.

XCMS calculates individual chromatographic peaks for each mzML file (retrieved using `xcms::chromPeaks(xcmsObj)`), these are then grouped together (using `xcms::groupChromPeaks`). Ideally the mzML files that contain the MS/MS spectra also contain sufficient MS1 scans for XCMS to detect MS1 chromatographic features. If this is the case, to determine if a MS2 spectra is to be linked to an XCMS grouped feature, the associated acquisition time of the MS/MS event has to be within the retention time window defined for the individual peaks associated for each file. The precursor m/z value also has to be within the user ppm tolerance to XCMS feature.

See below for representation of the linking (the * — * represent a many-to-many relationship) e.g. 1 or more MS/MS events can be linked to 1 or more individual feature and an individual XCMS feature can be linked to 1 or more grouped XCMS features

- [grouped XCMS feature - across files] * — * [individual XCMS feature - per file] * — * [MS/MS spectra]

Alternatively, if the "useGroup" argument is set to TRUE, the full width of the grouped peak (determined as the minimum `rtmin` and maximum `rtmax` of the all associated individual peaks) will be used. This option should be used if the mzML file with MS/MS has very limited MS1 data and so individual chromatographic peaks might not be detected with the mzML files containing the MS/MS data. However, it should be noted this may lead to potential inaccurate linking.

- [grouped XCMS peaks] * — * [MS/MS spectra]

Example LC-MS/MS processing workflow:

- Purity assessments
 - (mzML files) -> purityA -> (pa)
- XCMS processing
 - (mzML files) -> xcms.findChromPeaks -> (optionally) xcms.adjustRtime -> xcms.groupChromPeaks -> (xcmsObj)
 - — *Older versions of XCMS* — (mzML files) -> xcms.xcmsSet -> xcms.group -> xcms.retcor -> xcms.group -> (xcmsObj)
- Fragmentation processing
 - (xcmsObj, pa) -> **frag4feature** -> filterFragSpectra -> averageAllFragSpectra -> createDatabase -> spectralMatching -> (sqlite spectral database)

Additional notes:

- If using only a single file, then grouping still needs to be performed within XCMS before frag4feature can be used.
- Fragmentation spectra below a certain precursor ion purity can be removed (see plim argument).
- A SQLite database can be created directly here but the functionality has been deprecated and the createDatabase function should now be used
- Can experience some problems when using XCMS version < 3 and obiwrap retention time correction.

Usage

```
## S4 method for signature 'purityA'
frag4feature(
  pa,
  xcmsObj,
  ppm = 5,
  plim = NA,
  intense = TRUE,
  convert2RawRT = TRUE,
  useGroup = FALSE,
  createDb = FALSE,
  outDir = ".",
  dbName = NA,
  grpPeaklist = NA,
  use_group = NA,
  out_dir = NA,
  create_db = NA,
  grp_peaklist = NA,
  db_name = NA,
  xset = NA
)
```


Arguments

| | |
|---------------|--|
| pa | object; purityA object |
| xcmsObj | object; XCMSnExp, xcmsSet or xsAnnotate object derived from the same files as those used to create the purityA object |
| ppm | numeric; ppm tolerance between precursor mz and XCMS feature mz |
| plim | numeric; minimum purity of precursor to be included |
| intense | boolean; If TRUE the most intense precursor will be used. If FALSE the precursor closest to the center of the isolation window will be used |
| convert2RawRT | boolean; If retention time correction has been used in XCMS set this to TRUE |
| useGroup | boolean; Ignore individual peaks and just find matching fragmentation spectra within the (full) rtmin rtmax of each grouped feature |
| createDb | boolean; if yes, generate a database of MS2 spectra |
| outDir | string; path where (optionally generated) database file should be saved |
| dbName | character; name to assign to (optionally exported) database. |
| grpPeaklist | dataframe; Can use any peak dataframe to add to databse. Still needs to be derived from the "obj" object though |
| use_group | boolean; (Deprecated, to be removed - replaced with useGroup argument for style consistency) |
| out_dir | character; (Deprecated, to be removed - use createDatabase function) Path where database will be created |
| create_db | boolean; (Deprecated, to be removed - use createDatabase function) SQLite database will be created of the results |
| grp_peaklist | dataframe; (Deprecated, to be removed - use createDatabase function) Can use any peak dataframe to add to databse. Still needs to be derived from the xset object though |
| db_name | character; (Deprecated, to be removed - use createDatabase function) If create_db is TRUE, a custom database name can be used, default is a time stamp |
| xset | object; (Deprecated, to be removed - use xcmsObj) 'xcmsSet' object derived from the same files as those used to create the purityA object |

Value

Returns a purityA object (pa) with the following slots populated:

- pa@grp_d_f: A dataframe of the grouped XCMS features linked to the associated fragmentation spectra precursor details is recorded here
- pa@grp_ms2: A list of fragmentation spectra associated with each grouped XCMS feature is recorded here
- pa@f4f_link_type: The linking method is recorded here (e.g. individual peaks or grouped - "useGroup=TRUE")

Examples

```

library(xcms)
library(MSnbase)
library(magrittr)
##### XCMS #####
## Read in MS data
msmsPths <- list.files(system.file("extdata", "lcms", "mzML",
                                package="msPurityData"), full.names = TRUE, pattern = "MSMS")
ms_data = readMSData(msmsPths, mode = 'onDisk', msLevel. = 1)

## Find peaks in each file
cwp <- CentWaveParam(snthresh = 5, noise = 100, ppm = 10, peakwidth = c(3, 30))
xcmsObj <- xcms::findChromPeaks(ms_data, param = cwp)

## Optionally adjust retention time
xcmsObj <- adjustRtime(xcmsObj , param = ObiwrapParam(binSize = 0.6))

## Group features across samples
pdp <- PeakDensityParam(sampleGroups = c(1, 1), minFraction = 0, bw = 30)
xcmsObj <- groupChromPeaks(xcmsObj , param = pdp)

## Or if using the old XCMS functions
#xcmsObj <- xcms::xcmsSet(msmsPths)
#xcmsObj <- xcms::group(xcmsObj)
#xcmsObj <- xcms::retcor(xcmsObj)
#xcmsObj <- xcms::group(xcmsObj)

##### msPurity #####
pa <- purityA(msmsPths)
pa <- frag4feature(pa, xcmsObj)

```

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 mzmach.

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

```
datapath <- system.file("extdata", "dims", "mzML", package="msPurityData")
inDF <- Getfiles(datapath, 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)
grppeP <- 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 consisting 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)
grppeP <- 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% efficient)

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 | <i>Q-Exactive +/- 0.5 range, normalisation for isolation window efficiency</i> |
|------------|--|

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 than 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 +/- 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 | <i>Raised cosine normalisation for isolation window efficiency</i> |
|---------------|--|

Description

Creates a function based on a raised 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)
```

msPurity

msPurity *package*

Description

msPurity Bioconductor

Author(s)

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- Martin Jones [contributor]
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- Andris Jankevics [contributor]
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- Warwick Dunn [thesis advisor]

See Also

Useful links:

- <https://github.com/computational-metabolomics/msPurity/>
- Report bugs at <https://github.com/computational-metabolomics/msPurity/issues/new>

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 | <i>Assess the acquired precursor ion purity of MS/MS spectra (constructor)</i> |
|---------|--|

Description**General:**

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

The precursor ion purity represents the measure of the contribution of a selected precursor peak in an isolation window used for fragmentation and can be used as away of assessing the spectral quality and level of "contamination" of fragmentation spectra.

The calculation involves dividing the intensity of the selected precursor peak by the total intensity of the isolation window and is performed before and after the MS/MS scan of interest and interpolated at the recorded time of the MS/MS acquisition.

Additionally, isotopic peaks are annotated and omitted from the calculation, low abundance peaks are removed that are thought to have minor contribution to the resulting MS/MS spectra and the isolation efficiency of the mass spectrometer can be used to normalise the intensities used for the calculation.

The output is a purityA S4 class object (referred to as pa for convenience throughout the manual). The object contains a slot (pa@puritydf) where the details of the purity assessments for each MS/MS scan. The purityA object can then be used for further processing including linking the fragmentation spectra to XCMS features, averaging fragmentation, database creation and spectral matching (from the created database).

Example LC-MS/MS processing workflow:

The purityA object can be used for further processing including linking the fragmentation spectra to XCMS features, averaging fragmentation, database creation and spectral matching (from the created database). See below for an example workflow:

- Purity assessments
 - (mzML files) -> **purityA** -> (pa)
- XCMS processing
 - (mzML files) -> xcms.findChromPeaks -> (optionally) xcms.adjustRtime -> xcms.groupChromPeaks -> (xcmsObj)
 - — *Older versions of XCMS* — (mzML files) -> xcms.xcmsSet -> xcms.group -> xcms.retcor -> xcms.group -> (xcmsObj)
- Fragmentation processing
 - (xcmsObj, pa) -> frag4feature -> filterFragSpectra -> averageAllFragSpectra -> createDatabase -> spectralMatching -> (sqlite spectral database)

Isolation efficiency:

When the isolation efficiency of an MS instrument is known the peak intensities within an isolation window can be normalised for the precursor purity calculation. The isolation efficiency can be estimated by measuring a single precursor across a sliding window. See figure 3 from the original msPurity paper (Lawson et al 2017). This has been experimentally measured for a Thermo Fisher Q-Exactive Mass spectrometer using 0.5 Da windows and can be set within msPurity by using msPurity::iwNormQE.5() as the input to the iwNormFunc argument.

Other options to model the isolation efficiency the gaussian isolation window msPurity::iwNormGauss(minOff=-0.5, maxOff=0.5) or a R-Cosine window msPurity::iwNormRCosine(minOff=-0.5, maxOff=0.5). Where the minOff and maxOff can be altered depending on the isolation window size.

A user can also define their own normalisation function. The only requirement of the function is that given a value between the minOff and maxOff a normalisation value between 0-1 is returned.

Notes regarding instrument specific isolation window offsets used::

- The isolation widths offsets will be automatically determined from extracting metadata from the mzML file. However, for some vendors though this is not recorded, in these cases the offsets should be given by the user as an argument (offsets).
- 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,
  ppmInterp = 7
)

```

Arguments

| | |
|-------------|---|
| fileList | vector; mzML file paths |
| cores | numeric; Number of cores to use |
| mostIntense | boolean; True if the most intense peak is used for calculation. Set to FALSE if the peak closest to mz value detailed in mzML meta data. |
| nearest | boolean; True if the peak selected is from either the preceding scan or the nearest. |
| offsets | vector; Override the isolation offsets found in the mzML file e.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) |
| ppmInterp | numeric; Set the ppm tolerance for the precursor ion purity interpolation. i.e. the ppm tolerance between the precursor ion found in the neighbouring scans. |

Value

Returns a purityA object (pa) with the pa@puritydf slot updated

The purity dataframe (**pa@puritydf**) consists of the following columns:

- pid: unique id for MS/MS scan
- fileid: unique id for mzML file
- seqNum: scan number
- precursorIntensity: precursor intensity value as defined in the mzML file
- precursorMZ: precursor m/z value as defined in the mzML file
- precursorRT: precursor RT value as defined in the mzML file
- precursorScanNum: precursor scan number value as defined in mzML file
- id: unique id (redundant)
- filename: mzML filename
- precursorNearest: MS1 scan nearest to the MS/MS scan
- aMz: The m/z value in the "precursorNearest" MS1 scan which most closely matches the precursorMZ value provided from the mzML file
- aPurity: The purity score for aMz
- apkNm: The number of peaks in the isolation window for aMz
- iMz: The m/z value in the precursorNearest MS1 scan that is the most intense within the isolation window.
- iPurity: The purity score for iMz
- ipkNm: The number of peaks in the isolation window for iMz
- inPurity: The interpolated purity score (the purity score is calculated at neighbouring MS1 scans and interpolated at the point of the MS/MS acquisition)
- inpkNm: The interpolated number of peaks in the isolation window

The remaining slots for purityA class include

- pa@cores: The number of CPUs to be used for any further processing with this purityA object
- pa@fileList: list of the mzML files that have been processed
- pa@mzRback: The backend library used by mzR to extract information from the mzML file (e.g. pwiz)
- pa@grpед_df: If frag4feature has been performed, a dataframe of the grouped XCMS features linked to the associated fragmentation spectra precursor details is recorded here
- pa@grpед_ms2: If frag4feature has been performed, a list of fragmentation spectra associated with each grouped XCMS feature is recorded here
- pa@f4f_link_type: If frag4feature has been performed, the 'linking method' is recorded here, e.g. 'group' or 'individual'. Default is 'individual', see frag4feature documentation for more details
- pa@av_spectra: if averageIntraFragSpectra, averageInterFragSpectra, or averageAllFragSpectra have been performed, the average spectra is recorded here

- pa@av_intra_params: If averageIntraFragSpectra has been performed, the parameters are recorded here
- pa@av_inter_params: if averageInterFragSpectra has been performed, the parameters are recorded here]
- pa@av_all_params: If averageAllFragSpectra has been performed, the parameters are recorded here
- pa@db_path: If create_database has been performed, the resulting path to the database is recorded here

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 obiwrap) |
| 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, pattern =
xset <- readRDS(system.file("extdata", "tests", "xcms", "ms_only_xset_OLD.rds", package="msPurity"))
xset@filepaths[1] <- msPths[basename(msPths)=="LCMS_1.mzML"]
xset@filepaths[2] <- msPths[basename(msPths)=="LCMS_2.mzML"]
px <- purityX(xset, singleFile = 1)
```

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

Description

General

Perform spectral matching to spectral libraries for an LC-MS/MS dataset.

The spectral matching is performed from a **Query** SQLite spectral-database against a **Library** SQLite spectral-database.

The SQLite schema of the spectral database can be detailed Schema details can be found [here](#).

The query spectral-database in most cases should contain be the "unknown" spectra database generated the msPurity function createDatabase as part of a msPurity-XCMS data processing workflow.

The library spectral-database in most cases should contain the "known" spectra from either public or user generated resources. The library SQLite database by default contains data from MoNA including Massbank, HMDB, LipidBlast and GNPS. A larger database can be downloaded from [here](#). To create a user generated library SQLite database the following tool can be used to generate a SQLite database from a collection of MSP files: [msp2db](#). It should be noted though, that as long as the schema of the spectral-database is as described [here](#), then any database can be used for either the library or query - even allowing for the same database to be used.

The spectral matching functionality has four main components, spectral filtering, spectral alignment, spectral matching, and summarising the results.

Spectral filtering is simply filtering both the library and query spectra to be search against (e.g. choosing the library source, instrument, retention time, precursor PPM tolerance etc).

The spectral alignment stage involves aligning the query peaks to the library peaks. The approach used is similar to modified pMatch algorithm described in Zhou et al 2015.

The spectral matching of the aligned spectra is performed against a combined intensity and m/z weighted vector - created for both the query and library spectra (wq and wl). See below:

$$w = intensity^x * mz^y$$

Where x and y represent weight factors, defaults to x=0.5 and y=2 as per MassBank. These can be adjusted by the user though.

The aligned weighted vectors are then matched using dot product cosine, reverse dot product cosine and the composite dot product. See below for dot product cosine equation.

$$dpc = wq * wl / \sqrt{\sum wq^2} * \sqrt{\sum wl^2}$$

See the vignettes for more details regarding matching algorithms used.

Example LC-MS/MS processing workflow

- Purity assessments
 - (mzML files) -> purityA -> (pa)

- XCMS processing
 - (mzML files) -> xcms.findChromPeaks -> (optionally) xcms.adjustRtime -> xcms.groupChromPeaks -> (xcmsObj)
 - — *Older versions of XCMS* — (mzML files) -> xcms.xcmsSet -> xcms.group -> xcms.retcor -> xcms.group -> (xcmsObj)
- Fragmentation processing
 - (xcmsObj, pa) -> frag4feature -> filterFragSpectra -> averageAllFragSpectra -> create-Database -> **spectralMatching** -> (sqlite spectral database)

Usage

```
spectralMatching(
  q_dbPth,
  l_dbPth = NA,
  q_purity = NA,
  q_ppmProd = 10,
  q_ppmPrec = 5,
  q_raThres = NA,
  q_pol = NA,
  q_instrumentTypes = NA,
  q_instruments = NA,
  q_sources = NA,
  q_spectraTypes = c("av_all", "inter"),
  q_pids = NA,
  q_rtrange = c(NA, NA),
  q_spectraFilter = TRUE,
  q_xcmsGroups = NA,
  q_accessions = NA,
  l_purity = NA,
  l_ppmProd = 10,
  l_ppmPrec = 5,
  l_raThres = NA,
  l_pol = "positive",
  l_instrumentTypes = NA,
  l_instruments = NA,
  l_sources = NA,
  l_spectraTypes = NA,
  l_pids = NA,
  l_rtrange = c(NA, NA),
  l_spectraFilter = FALSE,
  l_xcmsGroups = NA,
  l_accessions = NA,
  usePrecursors = TRUE,
  raW = 0.5,
  mzW = 2,
  rttol = NA,
  q_dbType = "sqlite",
  q_dbName = NA,
```

```

q_dbHost = NA,
q_dbUser = NA,
q_dbPass = NA,
q_dbPort = NA,
l_dbType = "sqlite",
l_dbName = NA,
l_dbHost = NA,
l_dbUser = NA,
l_dbPass = NA,
l_dbPort = NA,
cores = 1,
updateDb = FALSE,
copyDb = FALSE,
outPth = "sm_result.sqlite"
)

```

Arguments

| | |
|-------------------|---|
| q_dbPth | character; Path of the database of queries that will be searched against the library spectra. Generated from createDatabase |
| l_dbPth | character; path to library spectral SQLite database. Defaults to msPurityData package data. |
| q_purity | character; Precursor ion purity threshold for the query spectra |
| q_ppmProd | numeric; ppm tolerance for query product |
| q_ppmPrec | numeric; ppm tolerance for query precursor |
| q_raThres | numeric; Relative abundance threshold for query spectra |
| q_pol | character; Polarity of query spectra ('positive', 'negative', NA). |
| q_instrumentTypes | vector; Instrument types for query spectra. |
| q_instruments | vector; Instruments for query spectra (note that this is used in combination with q_instrumentTypes - any spectra matching either q_instrumentTypes or q_instruments will be used). |
| q_sources | vector; Sources of query spectra (e.g. massbank, hmdb). |
| q_spectraTypes | character; Spectra types of query spectra to perform spectral matching e.g. ('scan', 'av_all', 'intra', 'inter') |
| q_pids | vector; pids for query spectra (correspond to column 'pid' in s_peak_meta) |
| q_rtrange | vector; retention time range (in secs) of query spectra, first value minimum time and second value max e.g. c(0, 10) is between 0 and 10 seconds |
| q_spectraFilter | boolean; For query spectra, if prior filtering performed with msPurity, flag peaks will be removed from spectral matching |
| q_xcmsGroups | vector; XCMS group ids for query spectra |
| q_accessions | vector; accession ids to filter query spectra |
| l_purity | character; Precursor ion purity threshold for the library spectra (uses interpolated purity - inPurity) |

| | |
|-------------------|---|
| l_ppmProd | numeric; ppm tolerance for library product |
| l_ppmPrec | numeric; ppm tolerance for library precursor |
| l_raThres | numeric; Relative abundance threshold for library spectra |
| l_pol | character; Polarity of library spectra ('positive', 'negative', NA) |
| l_instrumentTypes | vector; Instrument types for library spectra. |
| l_instruments | vector; Instruments for library spectra (note that this is used in combination with q_instrumentTypes - any spectra matching either q_instrumentTypes or q_instruments will be used). |
| l_sources | vector; Sources of library spectra (e.g. massbank, hmdb). |
| l_spectraTypes | vector; Spectra type of library spectra to perform spectral matching with e.g. ('scan', 'av_all', 'intra', 'inter') |
| l_pids | vector; pids for library spectra (correspond to column 'pid' in s_peak_meta) |
| l_rtrange | vector; retention time range (in secs) of library spectra, first value minimum time and second value max e.g. c(0, 10) is between 0 and 10 seconds |
| l_spectraFilter | boolean; For library spectra, if prior filtering performed with msPurity, flag peaks will be removed from spectral matching |
| l_xcmsGroups | vector; XCMS group ids for library spectra |
| l_accessions | vector; accession ids to filter library spectra |
| usePrecursors | boolean; If TRUE spectra will be filtered by similarity of precursors based on ppm range defined by l_ppmPrec and q_ppmPrec |
| raW | numeric; Relative abundance weight for spectra (default to 0.5 as determined by massbank for ESI data) |
| mzW | numeric; mz weight for spectra (default to 2 as determined by massbank for ESI data) |
| rttol | numeric ; Tolerance in time range between the library and query spectra retention time |
| q_dbType | character; Query database type for compound database can be either (sqlite, postgres or mysql) |
| q_dbName | character; Query database name (only applicable for postgres and mysql) |
| q_dbHost | character; Query database host (only applicable for postgres and mysql) |
| q_dbUser | character; Query database user (only applicable for postgres and mysql) |
| q_dbPass | character; Query database pass - Note this is not secure! use with caution (only applicable for postgres and mysql) |
| q_dbPort | character; Query database port (only applicable for postgres and mysql) |
| l_dbType | character; Library database type for compound database can be either (sqlite, postgres or mysql) |
| l_dbName | character; Library database name (only applicable for postgres and mysql) |
| l_dbHost | character; Library database host (only applicable for postgres and mysql) |
| l_dbUser | character; Library database user (only applicable for postgres and mysql) |

| | |
|----------|---|
| l_dbPass | character; Library database pass - Note this is not secure! use with caution (only applicable for postgres and mysql) |
| l_dbPort | character; Library database port (only applicable for postgres and mysql) |
| cores | numeric; Number of cores to use |
| updateDb | boolean; Update the Query SQLite database with the results |
| copyDb | boolean; If updating the database - perform on a copy rather than the original query database |
| outPth | character; If copying the database - the path of the new database file |

Value

Returns a list containing the following elements

q_dbPth

Path of the query database (this will have been updated with the annotation results if updateDb argument used)

xcmsMatchedResults

If the query spectra had XCMS based chromatographic peaks tables (e.g c_peak_groups, c_peaks) in the sqlite database - it will be possible to summarise the matches for each XCMS grouped feature. The dataframe contains the following columns

- lpid - id in database of library spectra
- qpId - id in database of query spectra
- dpc - dot product cosine of the match
- rdpc - reverse dot product cosine of the match
- cdpc - composite dot product cosine of the match
- mcount - number of matching peaks
- allcount - total number of peaks across both query and library spectra
- mpercent - percentage of matching peaks across both query and library spectra
- library_rt - retention time of library spectra
- query_rt - retention time of query spectra
- rtdiff - difference between library and query retention time
- library_precursor_mz - library precursor mz
- query_precursor_mz - query precursor mz
- library_precursor_ion_purity - library precursor ion purity
- query_precursor_ion_purity - query precursor ion purity
- library_accession - library accession value (unique string or number given to either MoNA or Massbank data entries)
- library_precursor_type - library precursor type (i.e. adduct)
- library_entry_name - Name given to the library spectra
- inchikey - inchikey of the matched library spectra

- library_source_name - source of the spectra (e.g. massbank, gnps)
- library_compound_name - name of compound spectra was obtained from

matchedResults

All matched results from the query spectra to the library spectra. Contains the same columns as above but without the XCMS details. This table is useful to observe spectral matching results for all MS/MS spectra irrespective of if they are linked to XCMS MS1 features.

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

Examples

```
##### XCMS #####
## Read in MS data
#msmsPths <- list.files(system.file("extdata", "lcms", "mzML",
#                               package="msPurityData"), full.names = TRUE, pattern = "MSMS")
#ms_data = readMSData(msmsPths, mode = 'onDisk', msLevel. = 1)

## Find peaks in each file
#cwp <- CentWaveParam(snthresh = 5, noise = 100, ppm = 10, peakwidth = c(3, 30))
#xcmsObj <- xcms::findChromPeaks(ms_data, param = cwp)

## Optionally adjust retention time
#xcmsObj <- adjustRtime(xcmsObj , param = ObiwrapParam(binSize = 0.6))

## Group features across samples
#pdp <- PeakDensityParam(sampleGroups = c(1, 1), minFraction = 0, bw = 30)
#xcmsObj <- groupChromPeaks(xcmsObj , param = pdp)

##### msPurity #####
#pa <- purityA(msmsPths)
#pa <- frag4feature(pa = pa, xcmsObj = xcmsObj)
#pa <- filterFragSpectra(pa, allfrag=TRUE)
#pa <- averageAllFragSpectra(pa)
#q_dbPth <- createDatabase(pa, xcmsObj, metadata=list('polarity'='positive', 'instrument'='Q-Exactive'))
#sm_result <- spectralMatching(q_dbPth, cores=4, l_pol='positive')

td <- tempdir()
q_dbPth <- system.file("extdata", "tests", "db", "createDatabase_example.sqlite", package="msPurity")

rid <- paste0(paste0(sample(LETTERS, 5, TRUE), collapse=""), paste0(sample(9999, 1, TRUE), collapse=""), ".sqlite")
sm_out_pth <- file.path(td, rid)

result <- spectralMatching(q_dbPth, q_xcmsGroups = c(53, 89, 410), cores=1, l_accessions = c('PR100407', 'ML005101'),
                           q_spectraTypes = 'av_all',
                           updateDb = TRUE,
                           copyDb = TRUE,
                           outPth = sm_out_pth)
```

| | |
|-------------------|-------------------------------------|
| spectral_matching | <i>Spectral matching deprecated</i> |
|-------------------|-------------------------------------|

Description

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

msPurity::spectral_matching is deprecated - please use msPurity::spectralMatching for future use

Usage

```
spectral_matching(  
  query_db_pth,  
  ra_thres_l = 0,  
  ra_thres_q = 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 = ".",  
  ra_w = 0.5,  
  mz_w = 2,  
  spectra_type_q = "scans",  
  ra_thres_t = NA,  
  target_db_pth = NA,  
  rt_range = c(NA, NA),  
  rttol = NA,  
  match_alg = "dpc"  
)
```

Arguments

| | |
|--------------|---|
| query_db_pth | character; Path of the database of targets (queries) 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_q | numeric; Relative abundance threshold for target (query) 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 [optional]; If target_db_pth set to NA, a new database can be created using pa, xset and grp_peaklist |
| xset | xcms object [optional]; If target_db_pth set to NA, a new database can be created using pa, xset and grp_peaklist |
| grp_peaklist | dataframe [optional]; If target_db_pth set to NA, a new database can be created using pa, xset and grp_peaklist |
| out_dir | character [optional]; If target_db_pth set to NA, Out directory for the SQLite result database |
| ra_w | numeric; Relative abundance weight for spectra |
| mz_w | numeric; mz weight for spectra |
| spectra_type_q | character; Type of fragmentation spectra from query to match with "scans" = all individual scans, "av_intra" = averaged spectra (intra), "av_inter" = averaged spectra (inter), "av_all" = averaged all spectra ignoring inter-intra relationships |
| ra_thres_t | numeric [deprecated]; The relative abundance threshold for the query spectra (use ra_thres_q for future use) |
| target_db_pth | character [deprecated]; The query database path (use query_db_pth for future use) |
| rt_range | vector [optional]; Vector of retention time range to filter the library spectra (rtmin, rtmax). Default is to ignore retention time range |
| rttol | numeric [optional]; Tolerance in time range between the Library and Query database retention time (in seconds) NA to ignore |
| match_alg | character; Can either use dot product cosine (dpc) or match factor (mf) for spectral matching. Defaults to dpc |

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,
#                               pattern = "MSMS")
#xset <- xcms::xcmsSet(msmsPths)
#xset <- xcms::group(xset)
#xset <- xcms::retcor(xset)
#xset <- xcms::group(xset)

#pa <- purityA(msmsPths)
#pa <- frag4feature(pa, xset)
#pa <- averageAllFragSpectra(pa)
#db_pth <- create_database(pa, xset)
#q_dbPth <- system.file("extdata", "tests", "db",
#                      "create_database_example.sqlite", package="msPurity")
#result <- spectral_matching(q_dbPth, spectra_type_q="av_all")
```

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 corresponding 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

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