CAMERA

April 20, 2011

`annotateDiffreport` *Deconvolute/Annotate LC/ESI-MS data*

Description

Wrapper function for the xcms diffreport and the annotate function. Returns a diffreport with the result from the annotation progress.

Usage

```
annotateDiffreport(object, sample=NA, sigma = 6, perfwhm = 0.6, cor_eic_th = 0.7
                   multiplier = 3, polarity = "positive", nSlaves = 1, psg_list =
                   rules = NULL,class1 = levels(sampclass(object))[1], class2 = le
                   eicmax = 0, eicwidth = 200, sortpval = TRUE, classeic = c(class
                    metlin = FALSE, h = 480, w = 640, ...)
```

Arguments

`object`	xcmsSet with peak group assignments
`sample`	Index of which sample is used for the correlation, NA for auto-selection
`sigma`	Isotopic peak relationship table
`perfwhm`	Adduct/Fragment peak relationship table
`cor_eic_th`	correlation threshold (0..1)
`maxcharge`	max charge of the ions
`maxiso`	max number of isotopes
`ppm`	ppm error
`mzabs`	absolut error
`multiplier`	max. number n of [nM+x] clusterions
`polarity`	Which polarity mode was used for measuring of the ms sample
`nSlaves`	Number of slaves for parallel calculation (Warning: Beta)
`psg_list`	Index-list of pseudospectra. Only for those ones will the annotation be calculated. Useful as a speed-up
`pval_th`	pval threshold. Creates a new psg_list. A pseudospectra is selected if it contains peaks, with pval < pval_th

fc_th	Same as pval. Select those groups with contains peaks with fold-change > fc_th. Pval_th and fc_th can be combined
quick	If quick is TRUE, only groupFWHM and findIsotopes will be calculated. Useful for preselecting groups with psg_list
rules	User defined ruleset
class1	character vector with the first set of sample classes to be compared
class2	character vector with the second set of sample classes to be compared
filebase	base file name to save report, .tsv file and _eic will be appended to this name for the tabular report and EIC directory, respectively. if blank nothing will be saved
eicmax	number of the most significantly different analytes to create EICs for
eicwidth	width (in seconds) of EICs produced
sortpval	logical indicating whether the reports should be sorted by p-value
classeic	character vector with the sample classes to include in the EICs
value	intensity values to be used for the diffreport. If value="into", integrated peak intensities are used. If value="maxo", maximum peak intensities are used. If value="intb", baseline corrected integrated peak intensities are used (only available if peak detection was done by findPeaks.centWave).
metlin	mass uncertainty to use for generating link to Metlin metabolite database. the sign of the uncertainty indicates negative or positive mode data for M+H or M-H calculation. a value of FALSE or 0 removes the column
h	Numeric variable for the height of the eic and boxplots that are printed out.
w	Numeric variable for the width of the eic and boxplots print out made.
...	optional arguments to be passed to mt.teststat

Details

Batch script wrapper for combining the annotation and the diffreport for a (grouped) xcmsSet xs. Function list: 1: diffreport(), 2: groupFWHM(), 3: findIsotopes(), 4: groupCorr(), 5: findAdducts() For a speedup calculation users can create a quick run, with quick = TRUE to preselect pseudospectra of interest. The indices of those pseudospectra are set with psg_list in a second run. On the other hand, a automatic selection with pval_th and/or fc_th can be performed. Returns the normal xcms diffreport table, with the additional CAMERA slots

Value

annotate returns an xsAnnotate object. For more information about see xsAnnotate-class

Author(s)

Carsten Kuhl <ckuhl@ipb-halle.de>

Examples

```
#Multiple sample
library(CAMERA)
library(faahKO)
xs.grp     <- group(faahko)
```

```
xs.fill    <- fillPeaks(xs.grp)

#fast preselection
diffreport  <- annotateDiffreport(xs.fill,quick=TRUE)
index <- c(1,18,35,45,56) #Make only for those grps a adduct annotation
diffreport2 <- annotateDiffreport(xs.fill,psg_list=index)

#automatic selection, all groups with peaks p-val < 0.05 and fold-change > 3
diffreport <- annotateDiffreport(xs.fill,pval_th=0.05,fc=3)
```

`annotate` *Deconvolute/Annotate LC/ESI-MS data*

Description

Annotate isotope peaks, adducts and fragments for a (grouped) xcmsSet `xs`. Returns a xsAnnotate object.

Usage

```
annotate(object, sigma = 6, perfwhm = 0.6, cor_eic_th = 0.75, maxcharge = 3, max
```

Arguments

`object`	xcmsSet with peak group assignments
`sigma`	Isotopic peak relationship table
`perfwhm`	Adduct/Fragment peak relationship table
`cor_eic_th`	correlation threshold (0..1)
`maxcharge`	max charge of the ions
`maxiso`	max number of isotopes
`ppm`	ppm error
`mzabs`	absolut error
`multiplier`	max. number n of [nM+x] clusterions
`sample`	Index of which sample is used for the correlation, NA for auto-selection
`quick`	Use only groupFWHM and findIsotopes
`psg_list`	Calculation will only be done for the selected groups
`polarity`	Which polarity mode was used for measuring of the ms sample
`nSlaves`	Number of slaves for parallel calculation (Warning: Beta)
`max_peaks`	If run in parallel mode, value defines how much peaks will be calculated in every thread

Details

Batch script for a annotation for a (grouped) xcmsSet `xs`. Generate intern a xsAnnotate object and calls the member function for the annotation step. Function list: 1: groupFWHM() , 2: findIsotopes() , 3: groupCorr(), 4: findAdducts() Return the xsAnnotate object which all the annotations. For more information see the funtion manpages.

Value

`annotate` returns an xsAnnotate object. For more information about see xsAnnotate-class

Author(s)

Carsten Kuhl <ckuhl@ipb-halle.de>

Examples

```
library(CAMERA)
file <- system.file('mzdata/MM14.mzdata', package = "CAMERA")
xs   <- xcmsSet(file, method="centWave", ppm=30, peakwidth=c(5,10))
xsa  <- annotate(xs)
```

---

findAdducts-methods

Calculate Adducts and Annotate LC/ESI-MS Spectra

Description

Annotate adducts (and fragments) for a xsAnnotate object. Returns a xsAnnotate object with annotated pseudospectra.

Usage

```
findAdducts(object, ppm=5, mzabs=0.015, multiplier=3, polarity=NULL, rules=NULL
```

Arguments

`object`	the `xsAnnotate` object
`ppm`	ppm error for the search
`mzabs`	allowed variance for the search
`multiplier`	highest number(n) of allowed clusterion [nM+ion]
`polarity`	Which polarity mode was used for measuring of the ms sample
`rules`	personal ruleset or with NULL standard ruleset will be calculated
`max_peaks`	If run in parralel mode, this number defines how much peaks will be calculated in every thread
`psg_list`	Vector of pseudospectra indices. The correlation analysis will be only done for those groups

Details

Adducts (and fragments) are annotated for a xsAnnotate object. For every pseudospectra group, generated bei groupFWHM and groupCorr, all possible Adducts are calculated and mapped to the peaks. If at least two adducts match, a possible molecule-mass for the group can be calculated. After the annotation every masshypothese is checked against the charge of the calculated isotopes. It is recommend to call findIsotopes() before the annotation step.

Author(s)

Carsten Kuhl <ckuhl@ipb-halle.de>

Examples

```
 library(CAMERA)
 file <- system.file('mzdata/MM14.mzdata', package = "CAMERA")
 xs   <- xcmsSet(file, method="centWave", ppm=30, peakwidth=c(5,10))
 an   <- xsAnnotate(xs)
 an   <- groupFWHM(an)
 an <- findIsotopes(an)  # optional but recommended.
# an <- groupCorr(an) # optional but very recommended step
 an <- findAdducts(an,polarity="positive")
 peaklist <- getPeaklist(an) # get the annotated peak list
```

---

findIsotopes-methods

Deconvolute/Annotate LC/ESI-MS data

Description

Annotate isotope peaks for a xsAnnotate object. Returns a xsAnnotate object with annotated isotopes.

Arguments

`object`	the `xsAnnotate` object
`maxcharge`	max. number of the isotope charge
`maxiso`	max. number of the isotope peaks
`ppm`	ppm error for the search
`mzabs`	allowed variance for the search

Details

Isotope peaks are annotated for a xsAnnotate object according to given rules (maxcharge, maxiso). The algorithm benefits from a earlier grouping of the data, with groupFWHM. Generates a list of all possible isotopes, which is stored in object@isotopes. Those isotope information will be used in the groupCorr funtion.

Methods

object = "xsAnnotate" `findIsotopes(object, maxcharge=3, maxiso=3, ppm=5, mzabs=0.01)`

Author(s)

Carsten Kuhl <ckuhl@ipb-halle.de>

Examples

```
library(CAMERA)
file <- system.file('mzdata/MM14.mzdata', package = "CAMERA")
xs   <- xcmsSet(file, method="centWave", ppm=30, peakwidth=c(5,10))
an   <- xsAnnotate(xs)
an   <- groupFWHM(an)
an   <- findIsotopes(an)
```

---

findNeutralLoss *Find pseudospectra that contains a specific neutral loss*

Description

The method searches in every pseudospectra for a distance between two ions matching a provided mass difference. It returns a xcmsSet object containing the matching peaks.

Usage

```
findNeutralLoss(object, mzdiff=NULL, mzabs=0, mzppm=10)
```

Arguments

object	xsAnnotate object
mzdiff	neutral loss in Dalton
mzabs	absolut allowed mass difference
mzppm	relative allowed mass difference

Details

The function needs a xsAnnotate object after groupCorr or groupFWHM. The resulting object is a artificial xcmsSet, where the peaks with the specific neutral loss are stored in xcmsSet@peaks.

Author(s)

Carsten Kuhl <ckuhl@ipb-halle.de>

Examples

```
library(CAMERA)
file <- system.file('mzdata/MM14.mzdata', package = "CAMERA")
xs   <- xcmsSet(file, method="centWave", ppm=30, peakwidth=c(5,10))
an   <- xsAnnotate(xs)
an   <- groupFWHM(an)
xs.pseudo <- findNeutralLoss(an,mzdiff=18.01,mzabs=0.01) #Searches for Peaks with water
xs.pseudo@peaks #show Hits
```

findNeutralLossSpecs *Find pseudospectra that contains a specific neutral loss*

Description

The method searches in every pseudospectra for a distance between two ions matching a provided mass difference. It returns a boolean vector with the length equals to the number of pseudospectra, where a hit is marked with TRUE.

Usage

```
findNeutralLossSpecs(object, mzdiff=NULL, mzabs=0, mzppm=10)
```

Arguments

object	xsAnnotate object
mzdiff	neutral loss in Dalton
mzabs	absolut allowed mass difference
mzppm	relative allowed mass difference

Details

The function needs a xsAnnotate object after groupCorr or groupFWHM.

Author(s)

Carsten Kuhl <ckuhl@ipb-halle.de>

Examples

```
library(CAMERA)
file <- system.file('mzdata/MM14.mzdata', package = "CAMERA")
xs   <- xcmsSet(file, method="centWave", ppm=30, peakwidth=c(5,10))
an   <- xsAnnotate(xs)
an   <- groupFWHM(an)
hits <- findNeutralLossSpecs(an,mzdiff=18.01,mzabs=0.01) #Searches for Pseudspecta with
```

getIsotopeCluster *Retrieve the annotatad isotopes*

Description

Extract all annotated isotope cluster. Returns a list with one element per cluster. A element contains the charge of the molecule and a peakmatrix with mz and intensity value.

Usage

```
getIsotopeCluster(object, number=NULL, value="maxo")
```

Arguments

object	xsAnnotate object
number	Set to NULL extract all isotope cluster or to specific choosen ones
value	Which intensity values should be extracted. Allowed values are: maxo, into, intb

Details

This method extract the isotope annotation from a xsAnnotate object. The order of the resulting list is the same as the one in the peaklist. In the case of a multiple sample the intensity value for a peak is retrieved from the sample, which has been choosen for the pseudospectra in the grouping step.

Author(s)

Carsten Kuhl <ckuhl@ipb-halle.de>

Examples

```
  #single sample
  library(CAMERA)
  file <- system.file('mzdata/MM14.mzdata', package = "CAMERA")
  xs   <- xcmsSet(file, method="centWave", ppm=30, peakwidth=c(5,10))
  an   <- xsAnnotate(xs)
  an   <- groupFWHM(an)
  an   <- findIsotopes(an)
  isolist <- getIsotopeCluster(an)
  isolist[[10]] #get IsotopeCluster 10

  #multiple sample
  library(faahKO)
  xs <- group(faahko)
  xs <- fillPeaks(xs)
  an   <- xsAnnotate(xs)
  an   <- groupFWHM(an)
  an   <- findIsotopes(an)
  isolist <- getIsotopeCluster(an)

  ##Interaction with Rdisop
 ## Not run:
  library(Rdisop)
  isotopes.decomposed <- lapply(isolist,function(x) {
    decomposeIsotopes(x$peaks[,1],x$peaks[,2],z=x$charge);
  }) #decomposed isotope cluster, filter steps are recommended

## End(Not run)
```

---

getPeaklist *Retrieve the annotatad peaklist*

Description

Extract all information from an xsAnnotate object. Returns a peaklist with annotated peaks.

Usage

```
getPeaklist(object)
```

Arguments

object	xsAnnotate object

Details

This function extract the peaktable from an xsAnnotate object, containing three additional columns (isotopes, adducts, pseudospectrum) with represents the annotation results. For a grouped xcmsSet it returns the grouped peaktable.

Author(s)

Carsten Kuhl <ckuhl@ipb-halle.de>

Examples

```
library(CAMERA)
  file <- system.file('mzdata/MM14.mzdata', package = "CAMERA")
  xs   <- xcmsSet(file, method="centWave", ppm=30, peakwidth=c(5,10))
  an   <- xsAnnotate(xs)
  an   <- groupFWHM(an)
  an   <- findIsotopes(an)
  an   <- findAdducts(an,polarity="positive")
  peaklist <- getPeaklist(an)
```

---

getpspectra *Retrieve a spectra-group peaklist*

Description

Extract one group from a xsAnnotate object. Returns a peaklist with annotated peaks.

Usage

```
getpspectra(object,grp)
```

Arguments

object	xsAnnotate object
grp	index of pseudo-spectra-group

Details

xsAnnotate groups LC/MS Peaklist after there EIC correlation and FWHM. These function extract one of these so called "pseudo spectra groups" with include the peaklist with there annotations. The annotation depends on a before called findAdducts() (and findIsotopes()). Attention: The indices for the isotopes, are those from the whole peaklist. See `getPeaklist()`.

Author(s)

Carsten Kuhl <ckuhl@ipb-halle.de>

Examples

```
library(CAMERA)
file <- system.file('mzdata/MM14.mzdata', package = "CAMERA")
xs   <- xcmsSet(c(file), method="centWave", ppm=30, peakwidth=c(5,10))
an   <- xsAnnotate(xs)
an   <- groupFWHM(an)
peaklist <- getpspectra(an, 1)
```

---

groupCorr-methods *EIC correlation grouping of LC/ESI-MS data*

Description

Grouping the peaks after the correlation of the EICs into pseudospectragroups for a xsAnnotate object. Return a xsAnnotate object with group information.

Usage

```
groupCorr(object, cor_eic_th=0.75, psg_list = NULL, polarity = NA)
```

Arguments

`object`	The `xsAnnotate` object
`cor_eic_th`	Correlation threshold for the EIC correlation
`psg_list`	Vector of pseudospectra indices. The correlation analysis will be only done for those groups
`polarity`	Optional feature, that ensure that [M+H]+, [M+Na]+, [M+K]+ in pos. mode and [M-H]- [M+Cl]- ions in neg. mode will not be seperated in different groups

Details

The algorithm correlates the EIC of a every peak with all others, to find the peaks that belong to one substance. LC/MS data should grouped with groupFWHM first. This step reduce the runtime a lot and increased the number of correct classifications. If you perform the findIsotope step first, annotated isotopes will always be in the same group.

Author(s)

Carsten Kuhl <ckuhl@ipb-halle.de>

Examples

```
library(CAMERA)
file        <- system.file('mzdata/MM14.mzdata', package = "CAMERA");
xs          <- xcmsSet(file, method="centWave", ppm=30, peakwidth=c(5, 10));
an          <- xsAnnotate(xs);
an.group    <- groupFWHM(an);
an.iso      <- findIsotopes(an.group); #optional step
index       <- c(1,4); #Only group one and four will be calculate
an.grp.corr <- groupCorr(an.iso, psg_list=index, polarity="positive");

#For csv output
# write.csv(file="peaklist_with_isotopes.csv",getPeaklist(an))

#Multiple sample
library(faahKO)
xs.grp       <- group(faahko)

#With selected sample
xsa          <- xsAnnotate(xs.grp, sample=1)
xsa.group    <- groupFWHM(xsa)
xsa.iso      <- findIsotopes(xsa.group) #optional step
index        <- c(1,4) #Only group one and four will be calculate
xsa.grp.corr <- groupCorr(xsa.iso, psg_list=index, polarity="positive")

#With automatic selection
xsa.auto     <- xsAnnotate(xs.grp)
xsa.grp      <- groupFWHM(xsa.auto)
xsa.iso      <- findIsotopes(xsa.grp) #optional step
index        <- c(1,4) #Only group one and four will be calculate
xsa.grp.corr <- groupCorr(xsa.iso, psg_list=index, polarity="positive")
#Note: Group 1 and 4 have no subgroups
```

`groupFWHM-methods` *FWHM-Grouping of LC/ESI-MS data*

Description

Group peaks of one xsAnnotate object after the FWHM of there retentiontimes into pseudospectra-groups. Returns a xsAnnotate object with group information.

Usage

```
groupFWHM(object, sigma = 6 , perfwhm = 0.6)
```

Arguments

`object`	the `xsAnnotate` object
`sigma`	the multiplier of the standard deviation
`perfwhm`	percentage of the width of the FWHM

Details

Every peak who eluated at the same time as a selected peak, will be part of the group. Same time is defined about the Rt_med +/- FWHM * perfwhm. For single sample the selection of peaks starts at the most abundant and goes down the smaller ones. In a multiple sample set you can define a sample, that will be used for the process or use the automatic selection. This select the most abundant peak as an representative for every peak group. Peak group means here those ones from the xcms grouping. The FWHM (full width at half maximum) of a peak is estimated as FWHM = SD * 2.35. The calculation of the SD, the peak is assumpted as a normal distribution.

Author(s)

Carsten Kuhl <ckuhl@ipb-halle.de>

Examples

```
library(CAMERA)
#Single sample
file <- system.file('mzdata/MM14.mzdata', package = "CAMERA")
xs   <- xcmsSet(file, method="centWave", ppm=30, peakwidth=c(5,10))
an   <- xsAnnotate(xs)
an   <- groupFWHM(an)

#Multiple sample
library(faahKO)
xs   <- group(faahko)
#With selected sample
xs.anno  <- xsAnnotate(xs, sample=1)
xs.group <- groupFWHM(xs.anno)

#With automatic selection
xs.anno.auto  <- xsAnnotate(xs)
xs.group.auto <- groupFWHM(xs.anno.auto)
```

---

mm14 *Extract of marker mixture 14 LC/MS data*

Description

xcmsSet object containing quantitated LC/MS peaks from a marker mixture. The data is a centroided subset from 117-650 m/z and 271-302 seconds with 134 peaks. Positive ionization mode data in mzData file format.

Usage

```
data(mm14)
```

Format

The format is:

```
Formal class 'xcmsSet' [package "xcms"] with 8 slots
    @ peaks    : num [1:83, 1:11] 117 117 118 119 136
  .. ..- attr(*, "dimnames")=List of 2
  .. .. ..$ : NULL
  .. .. ..$ : chr [1:11] "mz" "mzmin" "mzmax" "rt"
  ..@ groups   : logi[0 , 0 ]
  ..@ groupidx : list()
  ..@ phenoData:'data.frame': 1 obs. of  1 variable:
  .. ..$ class: Factor w/ 1 level "mzdata": 1
  ..@ rt       :List of 2
  .. ..$ raw      :List of 1
  .. .. ..$ : num [1:112] 270 271 271 271 272 ...
  .. ..$ corrected:List of 1
  .. .. ..$ : num [1:112] 270 271 271 271 272 ...
  ..@ filepaths: chr "mzdata/MM14.mzdata"
  ..@ profinfo :List of 2
  .. ..$ method: chr "bin"
  .. ..$ step  : num 0.1
  ..@ polarity : chr(0)
```

Details

The corresponding raw mzData files are located in the mzData subdirectory of this package.

Author(s)

Carsten Kuhl <ckuhl@ipb-halle.de>

Source

http://doi:10.1186/1471-2105-9-504

References

Data originally reported in "Highly sensitive feature detection for high resolution LC/MS" BMC Bioinformatics; 2008; 9:504.

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plotEICs-methods *Plot extracted ion chromatograms from (multiple) Pseudospectra*

Description

Batch plot a list of extracted ion chromatograms to the current graphics device.

Arguments

`object`	the `xsAnnotate` object
`xraw`	`xcmsRaw` object underlying the the xsAnnotate
`maxlabel`	How many m/z labels to print
`sleep`	seconds to pause between plotting EICs
`...`	other graphical parameters

Value

None.

Methods

object = "xsAnnotate" `plotEICs(object, xraw, pspec=1:length(object@pspectra), maxlabel=0, sleep=0)`

Author(s)

Steffen Neumann, <sneumann@ipb-halle.de>

See Also

xsAnnotate-class, png, pdf, postscript,

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plotPsSpectrum-methods

Plot a Pseudospectrum

Description

Plot a pseudospectrum, with the most intense peaks labelled, to the current graphics device.

Arguments

object	the xsAnnotate object
pspec	ID of the pseudospectrum to print
log	Boolean, whether the log(intensity) should be shown
value	Which of a peak's intensities should be used
maxlabel	How many m/z labels to print
title	Main title of the Plot
mzrange	Which m/z range should plotted
sleep	Time (in seconds) to wait between successive Spectra, if multiple pspec are requested.

Value

None.

Methods

object = "xsAnnotate" `plotPsSpectrum(object, pspec=NULL, log=FALSE, value="maxo", maxlabel=0, title=NULL,mzrange=numeric() sleep=0)`

Author(s)

Steffen Neumann, <sneumann@ipb-halle.de>

See Also

xsAnnotate-class, png, pdf, postscript,

psDist-methods *Distance methods for xsAnnotate*

Description

The package xcms contains several methods for calculating a distance between two sets of peaks. the CAMERA method `psDist` is the generic wrapper to use these methods for processing two pseudospectra from two different xsAnnotate objects.

Arguments

`object1`	a xsAnnotate object with pseudospectra
`object2`	a xsAnnotate object with pseudospectra
`PSpec1`	index of pseudospectrum in object1
`PSpec2`	index of pseudospectrum in object2
`method`	method to use for distance calculation. See details.
`...`	mzabs, mzppm and parameters for the distance function.

Details

Different algorithms can be used by specifying them with the `method` argument. For example to use the "meanMZmatch" approach one would use: `specDist(object1, object2, pspectrum1, pspectrum2, method="meanMZmatch")`. This is also the default.

Further arguments given by `...` are passed through to the function implementing the `method`.

A character vector of *nicknames* for the algorithms available is returned by `getOption("BioC")$xcms$specDist`
If the nickname of a method is called "meanMZmatch", the help page for that specific method can be accessed with `?specDist.meanMZmatch`.

Value

`mzabs`	maximum absolute deviation for two matching peaks
`mzppm`	relative deviations in ppm for two matching peaks
`symmetric`	use symmetric pairwise m/z-matches only, or each match

Methods

object1 = "xsAnnotate" `specDist(object1, object2, pspectrum1, pspectrum2,method,...)`

Author(s)

Joachim Kutzera, <jkutzer@ipb-halle.de>

`xsAnnotate-class` *Class xsAnnotate, a class for annotate peak data*

Description

This class transforms a set of peaks from multiple LC/MS or GC/MS samples into a matrix of preprocessed data. It groups the peaks and does nonlinear retention time correction without internal standards. It fills in missing peak values from raw data. Lastly, it generates extracted ion chromatograms for ions of interest.

Objects from the Class

Objects can be created with the `xsAnnotate` constructor which gathers peaks from a set NetCDF files. Objects can also be created by calls of the form `new("xsAnnotate", ...)`.

Slots

`annoGrp`: Assignment of mass hypotheses to correlation groups

`annoID`: The assignemnt of peaks to the mass difference rule used

`derivativeIons`: List with annotation result for every peak

`formula`: Matrix containing putative sum formula (intended for future use)

`isoID`: Matrix containing IDs and additional of all annotated isotope peaks

`groupInfo`: (grouped) Peaktable with "into" values

`isotopes`: List with annotated isotopid results for every peak

`polarity`: A single string with the polarity mode of the peaks

`pspectra`: List contains all pseudospectra with there peak IDs

`psSamples`: List containing information with sample was sample was selecteted as representative (automatic selection)

`ruleset`: A dataframe describing the mass difference rules used for the annotion

`runParallel`: Flag if CAMERA runs in serial or parallel mode

`sample`: Number of the used xcmsSet sample (beforehand sample selection)

`xcmsSet`: The embedded xcmsSet

Methods

groupFWHM `signature(object = "xsAnnotate")`: group the peak data after the FWHM of the retention time

groupCorr `signature(object = "xsAnnotate")`: group the peak data after the correlation of the EICs

findIsotopes `signature(object = "xsAnnotate")`: search for possible isotopes in the spectra

findAdducts `signature(object = "xsAnnotate")`: search for possible adducts in the spectra

plotEICs `signature(object = "xsAnnotate")`: plot EICs of pseudospectra

Note

No notes yet.

Author(s)

Carsten Kuhl, <ckuhl@ipb-halle.de>

See Also

xsAnnotate

`xsAnnotate` *Constructor for a xsAnnotate object which one assigned xcmsSet object*

Description

This function handles the construction of xsAnnotate object. It extract the peaktable from a given xcmsSet, which is used for all further analysis. The xcmsSet can be a single sample or multiple sample experiment. Since some functions needs to go back into the raw data, the selection algorithm must be choosen for a multiple sample. CAMERA includes two different strategies: A fixed selection, which sample = index of sample, or the default automatic solution (sample = NA). The automatic solution chooses the best sample for a specifc groups called pseudospectrum, see groupFWHM and groupCorr.

Usage

```
xsAnnotate(xs = NULL,sample=NA, nSlaves = 1)
```

Arguments

`xs`	a `xcmsSet` object
`sample`	Index of the group xcmsSet sample, that is used for the EIC corelations step. For automatic selection don"t set a value.
`nSlaves`	For parallel mode set nSlaves higher than 1, but not higher than the number of cpu cores.

Value

A `xsAnnotate` object.

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See Also

xsAnnotate-class

Examples

```
library(faahKO)
xs <- group(faahko)
xs.anno <- xsAnnotate(xs, sample=1)
#With automatic selection
xs.anno.autoselect <- xsAnnotate(xs)
```

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