

CAMERA

October 25, 2011

annotate-methods *Automatic deconvolution/annotation of LC/ESI-MS data*

Description

Wrapper skript for automatic annotation of isotope peaks, adducts and fragments for a (grouped) xcmsSet xs. The function returns an xsAnnotate object.

Usage

```
annotate(object, sample=NA, nSlaves=1, sigma=6, perfwHM=0.6,
  cor_eic_th=0.75, graphMethod="hcs", pval=0.05, calcCiS=TRUE,
  calcIso=FALSE, calcCaS=FALSE, maxcharge=3, maxiso=4, minfrac=0.5,
  ppm=5, mzabs=0.015, quick=FALSE, psg_list=NULL, rules=NULL,
  polarity="positive", multiplier=3, max_peaks=100 ,intval="into")
```

Arguments

object	xcmsSet with peak group assignments
sample	xsAnnotate: Sample selection for grouped xcmsSet, see xsAnnotate-class
nSlaves	xsAnnotate: Use parallel CAMERA mode, require Rmpi
sigma	groupFWHM: multiplier of the standard deviation
perfwHM	groupFWHM: percentage of FWHM width
cor_eic_th	groupCorr: correlation threshold (0..1)
graphMethod	groupCorr: Method selection for grouping peaks after correlation analysis into pseudospectra
pval	groupCorr: significant correlation threshold
calcCiS	groupCorr: Use correlation inside samples for peak grouping
calcIso	groupCorr: Use isotopic relationship for peak grouping
calcCaS	groupCorr: Use correlation across samples for peak grouping
maxcharge	findIsotopes: max. ion charge
maxiso	findIsotopes: max. number of expected isotopes
minfrac	findIsotopes: The percentage number of samples, which must satisfy the C12/C13 rule for isotope annotation

ppm	General ppm error
mzabs	General absolut error in m/z
quick	Use only groupFWHM and findIsotopes
psg_list	Calculation will only be done for the selected groups
rules	findAdducts: User defined ruleset
polarity	findAdducts: Which polarity mode was used for measuring of the ms sample
multiplier	findAdducts: If no ruleset is provided, calculate ruleset with max. number n of [nM+x] clusterions
max_peaks	How much peaks will be calculated in every thread using the parallel mode
intval	General used intensity value (into, maxo, intb)

Details

Batch script for annotation of an (grouped) `xcmsSet` `xs`. Generates an `xsAnnotate` object by calling all involved functions for the annotation step. Function list: 1: `groupFWHM()`, 2: `findIsotopes()`, 3: `groupCorr()`, 4: `findAdducts()` Return the `xsAnnotate` object, which inherits all annotations. For more information about the parameters see the specific function manpages.

Value

`annotate` returns an `xsAnnotate` object. For more information about the `xsAnnotate` object 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)
```

annotateDiffreport *Automatic deconvolution/annotation of LC/ESI-MS data*

Description

Wrapper function for the `xcms` `diffreport` and the `annotate` function. Returns a `diffreport` within the annotation results.

Usage

```
annotateDiffreport(object, sample=NA, nSlaves=1, sigma=6, perfwfm=0.6,
  cor_eic_th=0.75, graphMethod="hcs", pval=0.05, calcCiS=TRUE,
  calcIso=FALSE, calcCaS=FALSE, maxcharge=3, maxiso=4, minfrac=0.5,
  ppm=5, mzabs=0.015, quick=FALSE, psg_list=NULL, rules=NULL,
  polarity="positive", multiplier=3, max_peaks=100, intval="into",
  pval_th = NULL, fc_th = NULL, sortpval=TRUE, ...)
```

Arguments

object	xcmsSet with peak group assignments
sample	xsAnnotate: Sample selection for grouped xcmsSet, see xsAnnotate-class
nSlaves	xsAnnotate: Use parallel CAMERA mode, require Rmpi
sigma	groupFWHM: multiplier of the standard deviation
perfwHM	groupFWHM: percentage of FWHM width
cor_eic_th	groupCorr: correlation threshold (0..1)
graphMethod	groupCorr: Method selection for grouping peaks after correlation analysis into pseudospectra
pval	groupCorr: significant correlation threshold
calcCiS	groupCorr: Use correlation inside samples for peak grouping
calcIso	groupCorr: Use isotopic relationship for peak grouping
calcCaS	groupCorr: Use correlation across samples for peak grouping
maxcharge	findIsotopes: max. ion charge
maxiso	findIsotopes: max. number of expected isotopes
minfrac	findIsotopes: The percentage number of samples, which must satisfy the C12/C13 rule for isotope annotation
ppm	General ppm error
mzabs	General absolut error in m/z
quick	Use only groupFWHM and findIsotopes
psg_list	Calculation will only be done for the selected groups
rules	findAdducts: User defined ruleset
polarity	findAdducts: Which polarity mode was used for measuring of the ms sample
multiplier	findAdducts: If no ruleset is provided, calculate ruleset with max. number n of [nM+x] clusterions
max_peaks	How much peaks will be calculated in every thread using the parallel mode
intval	General used intensity value (into, maxo, intb)
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
sortpval	Sort diffreport after pvalues
...	Diffreport parameters see diffreport

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

annotateDiffreport returns an diffreport, see [diffreport](#), within additional columns containing the annotation results.

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,metlin = TRUE)

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

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

Description

Calculate the correlation across samples. Filtering correlation with specific parameters and returns a correlation matrix.

Usage

```
calcCaS(object,corval=0.75, pval=0.05, intval="into")
```

Arguments

object	The xsAnnotate object
corval	Correlation threshold for positive hits
pval	P-Value threshold for significance level of correlation
intval	Selection of the intensity values that should be used in the correlation analysis. Can be into, maxo or intb.

Details

Calculate pearson correlation between the peak intensities over all samples. Afterwards use cor.test for returning only significant correlation. Returns only those correlation, which are above both threshold. Set corval and pval to 0 to get the unfiltered correlation matrix. If the object is pregrouped with groupFWHM, then the correlation is only calculated between peaks within a pseudospectrum. Otherwise between all peaks.

Value

A matrix with 4 columns:

x	peak index according to peaktable
y	peak index according to peaktable
cor	correlation value between peak x and peak y
ps	pseudospektrum index for both peaks

Author(s)

Carsten Kuhl <ckuhl@ipb-halle.de>

See Also

[calcCiS](#) [groupCorr](#) [xsAnnotate-class](#)

Examples

```
library(CAMERA)
#Multiple sample
library(faahKO)
xs.grp      <- group(faahko)
#create xsAnnotate object
xsa        <- xsAnnotate(xs.grp)
#generate pseudospectra
xsa.group  <- groupFWHM(xsa)
#calculate correlation
correlationMatrix <- calcCaS(xsa.group)
```

calcCiS-methods *Calculate peak distance matrix after EIC correlation*

Description

Processing an `xsAnnotate` object and correlates peak EIC curves from one pseudospectrum, using a precalculated EIC matrix ([getAllPeakEICs](#)). It return a weighted edge list as distance matrix between peaks according to the correlation analysis. The edge value is the pearson correlation coefficient. The list can be used as input for [calcPC](#).

Usage

```
calcCiS(object, EIC=EIC, corval=0.75, pval=0.05, psg_list=NULL)
```

Arguments

object	The <code>xsAnnotate</code> object
EIC	EIC Matrix
corval	Correlation threshold for the EIC correlation
pval	pvalue for testing correlation of significance
psg_list	Vector of pseudospectra indices. The correlation analysis will be only done for those 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. Only correlation with a higher value than the correlation threshold and significant p-values will be returned.

Value

A matrix with 4 columns:

x	peak index
y	peak index
cor	correlation value
ps	pseudospectrum index, which contains x and y

Author(s)

Carsten Kuhl <ckuhl@ipb-halle.de>

See Also

[calcCaS](#) [groupCorr](#) [getAllPeakEICs](#) [xsAnnotate-class](#)

calcIsotopes-methods

Calculate isotope distance matrix from xsAnnotate object

Description

Processing an xsAnnotate object with annotated isotopes ([findIsotopes](#)). It return a weighted edge list as distance matrix between peaks according to the isotope annotation. The edge value for recognized isotopes is 1 for all cases. The list can be used as input for [calcPC](#).

Arguments

object xsAnnotate object

Value

A matrix with 4 columns:

x	peak index
y	peak index
cor	edge value, always 1
ps	pseudospectrum index, which contains x and y

Methods

object = "xsAnnotate" calcIsotopes(object)

Author(s)

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

See Also

[calcPC xsAnnotate-class](#)

calcPC-methods

Peakclustering into pseudospectra according to a distance matrix

Description

A number of clustering methods exist in CAMERA. `calcPC` is the generic method.

Usage

```
calcPC(object, method, ...)
```

Arguments

<code>object</code>	xsAnnotate-class object
<code>method</code>	Method to use for clustering. See details.
<code>...</code>	Optional arguments to be passed along

Details

This algorithms cluster peaks from a `xsAnnotate` object into pseudospectra according to a provided distance matrix. Therefore all peaks are transformend into a graph, with peaks as nodes and the value from the distance matrix as edges. Afterwards a graph separation algorithm is applied, which searches in the graph for clusters. See the manpages of the specific clustering algorithms for more information.

If the `xsAnnotate` is pregrouped, for example [groupFWHM](#), only the already existing groups will be further processed.

The different algorithms that can be used by specifying them with the `method` argument. For example to use the highly connected subgraphs approach by E. Hartuv, R. Shamir, (1999), one would use: `calcPC(object, method="hcs")`. This is also the default, see [calcPC.hcs](#).

Further arguments given by `...` are passed through to the function implementing the `method`, which are most likely `ajc`. The parameter `ajc` is the peak distance matrix.

`getOption("BioC")$CAMERA$findPeaks.methods` returns a character vector of *nick-names* for the algorithms available.

The function returns a `xsAnnotate` object with grouping information, as list of peak indices. They are stored as `object@pspectra`.

See Also

[calcPC.lpc](#) [calcPC.hcs](#) [xsAnnotate-class](#)

calcPC.hcs	<i>Peakclustering into pseudospectra with the highly connected sub-graphs</i>
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Description

Cluster peaks from an `xsAnnotate` object into pseudospectra

Arguments

<code>object</code>	<code>xsAnnotate</code> object
<code>ajc</code>	Weighted symbolic edge list as four column matrix ("x","y","cor","ps"). Columns x,y are peak indices, cor the edge value and ps the pseudospectrum index, where both peaks occur.
<code>psg_list</code>	additional vector ps pseudospectra indices, which are used in the clustering. If set to NULL all pseudospectra will be processed.

Details

In some cases, is the peak grouping after retentiontime with `groupFWHM` not enough to separate co-elution compounds. Therefore `groupCorr` use additional correlation analysis to achieve a separation. `calcPC` is part of this approach, which takes the calculated weighted edge list and performs the graph clustering. It returns an `xsAnnotate` object with further separated pseudospectra.

Methods

```
object = "xsAnnotate" calcPC.hcs(object, ajc=NULL, psg_list=NULL)
```

Author(s)

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

See Also

[calcPC](#) [groupCorr](#) [highlyConnSG](#) [xsAnnotate-class](#)

calcPC.lpc	<i>Peakclustering into pseudospectra with the label-propagation-community</i>
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Description

Cluster peaks from an `xsAnnotate` object into pseudospectra

Arguments

object	xsAnnotate object
ajc	Weighted symbolic edge list as four column matrix ("x","y","cor","ps"). Columns x,y are peak indices, cor the edge value and ps the pseudospectrum index, where both peaks occur.
psg_list	additional vector ps pseudospectra indices, which are used in the clustering. If set to NULL all pseudospectra will be processed.

Details

In some cases, is the peak grouping after retentiontime with [groupFWHM](#) not enough to separate co-elution compounds. Therefore [groupCorr](#) use additional correlation analysis to achieve a separation. `calcPC` is part of this approach, which takes the calculated weighted edge list and performs the graph clustering. It returns an `xsAnnotate` object with further separated pseudospectra.

Methods

```
object = "xsAnnotate" calcPC.lpc(object, ajc=NULL, psg_list=NULL)
```

Author(s)

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

See Also

[calcPC](#) [groupCorr](#) [xsAnnotate-class](#) [label.propagation.community](#)

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, max_peaks=100, psg_list=NULL)
```

Arguments

object	the <code>xsAnnotate</code> 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 parallel 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 by `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 mass hypothesis is checked against the charge of the calculated isotopes. It is recommended 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

Deconvolute/Annotate LC/ESI-MS data

Description

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

Usage

```
findIsotopes(object, maxcharge=3, maxiso=4, ppm=5, mzabs=0.01, intval="maxo",
```

Arguments

object	the <code>xsAnnotate</code> 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
intval	choose intensity values for C12/C13 check. Allowed values are into, maxo, intb
minfrac	in case of multiple samples, percentage value of samples, which have to contain the correct C12/C13 ratio

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` function. The intensity of the C13 isotope peak is checked against the C12 of proper ratio. In the case of multiple sample, all samples will be tested. `Minfrac` describe the minimal percentage of samples, which must passed the test. If peaks are NA, then this sample is skipped and the ratio is (found correct C12/C13 ratio) / (samples containing C12 and C13 peak).

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

<code>object</code>	<code>xsAnnotate</code> object
<code>mzdiff</code>	neutral loss in Dalton
<code>mzabs</code>	absolut allowed mass difference
<code>mzppm</code>	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)
#Searches for Peaks with water loss
xs.pseudo <- findNeutralLoss(an,mzdiff=18.01,mzabs=0.01)
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)
#Searches for Pseudospectra with water loss
hits <- findNeutralLossSpecs(an, mzdiff=18.01, mzabs=0.01)
```

getAllPeakEICs	<i>Generate EIC information from raw data</i>
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Description

Generate EIC data out of the raw data, according to the peak peaker information.

Usage

```
getAllPeakEICs(object, index)
```

Arguments

object	The xsAnnotate object
index	Sample index vector, with the same length as the number of peaks. Encoding from with sample the peak should be extracted. If all peaks should be generated from the same sample set index = rep(sample index, peak count)

Details

The function extract from the raw data the EIC curves. Therefore all .netcdf, .mzdata etc. files must be accessible. It returns a list with two item.

Value

A list with items:

EIC	EIC Matrix with rows = number of peaks and columns = maxscans. It contains mostly NA values and only in that part, where a peak had been found, the intensity information.
scantimes	Scantimes of each sample

Author(s)

Carsten Kuhl <ckuhl@ipb-halle.de>

See Also

[xsAnnotate-class](#)

Examples

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

#create xsAnnotate object
xsa        <- xsAnnotate(xs.grp)
#generate pseudospectra
xsa.group  <- groupFWHM(xsa)

#calculate correlation
```

```
tmp <- getAllPeakEICs(xsa.group, index=rep(1, nrow(xsa.group@groupInfo)))
#extract EIC matrix
EIC.matrix <- tmp$EIC;
```

getIsotopeCluster *Retrieve the annotated 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 chosen 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, see [getPeaklist](#). In the case of a multiple sample the intensity value for a peak is retrieved from the sample, which has been chosen 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	<i>Generate the annotated peaklist</i>
-------------	--

Description

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

Usage

```
getPeaklist(object, intval="into")
```

Arguments

<code>object</code>	<code>xsAnnotate</code> object
<code>intval</code>	Choose intensity values. Allowed values are <code>into</code> , <code>maxo</code> , <code>intb</code>

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 peaklist of one or more pseudospectra*

Description

Extract group(s) from a xsAnnotate object. Returns a peaklist as matrix 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 or more of these so called "pseudo spectra groups" with include the peaklist with there annotations. The annotation depends on a before called findAdducts() (and findIsotopes()). Important: 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)
#For one group
peaklist <- getpspectra(an, 1)
#For two groups
peaklist <- getpspectra(an, c(1,2))
```

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

Description

Peak grouping after correlation information into pseudospectrum groups for an xsAnnotate object. Return an xsAnnotate object with grouping information.

Usage

```
groupCorr(object, cor_eic_th=0.75, pval=0.05, graphMethod="hcs",
calcIso = FALSE, calcCiS = TRUE, calcCaS = FALSE, psg_list=NULL, ...)
```

Arguments

object	The xsAnnotate object
cor_eic_th	Correlation threshold for EIC correlation
pval	p-value threshold for testing correlation of significance
graphMethod	Clustering method for resulting correlation graph. See calcPC for more details.
calcIso	Include isotope detection informationen for graph clustering
calcCiS	Calculate correlation inside samples
calcCaS	Calculate correlation accross samples
psg_list	Vector of pseudospectra indices. The correlation analysis will be only done for those groups
...	Additional parameter

Details

The algorithm calculates different informations for group peaks into so called pseudospectra. This pseudospectra contains peaks, with have a high correlation between each other. So far three different kind of information are available. Correlation of intensities across samples (need more than 3 samples), EIC correlation between peaks inside a sample and additional the informationen about recognized isotope cluster can be included. After calculation of all these informations, they are combined as edge value into a graph object. A following graph clustering algorithm separate the peaks (nodes in the graph) into the pseudospectra.

Author(s)

Carsten Kuhl <ckuhl@ipb-halle.de>

See Also

[calcCiS](#) [calcCaS](#) [calcPC](#) [xsAnnotate-class](#)

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 for using isotope information
an.grp.corr <- groupCorr(an.iso, calcIso=TRUE);

#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
xsa.grp.corr <- groupCorr(xsa.iso, calcIso=TRUE)
```

```

#With automatic selection
xsa.auto      <- xsAnnotate(xsa.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
#We use also correlation across sample
xsa.grp.corr  <- groupCorr(xsa.iso, psg_list=index, calcIso=TRUE, calcCaS=TRUE)
#Note: Group 1 and 4 have no subgroups

```

groupFWHM

FWHM-Grouping of LC/ESI-MS data

Description

Group peaks of a `xsAnnotate` object according to their retention time into pseudospectra-groups. Uses the peak FWHMs as grouping borders. Returns `xsAnnotate` object with pseudospectra information.

Usage

```
groupFWHM(object, sigma = 6 , perfwhm = 0.6, intval = "maxo")
```

Arguments

<code>object</code>	the <code>xsAnnotate</code> object
<code>sigma</code>	the multiplier of the standard deviation
<code>perfwhm</code>	percentage of the width of the FWHM
<code>intval</code>	intensity values for ordering. Allowed values are <code>into</code> , <code>maxo</code> , <code>intb</code>

Details

Every peak who eluate at the same time-point as a selected peak, will be part of the group. Same time-point is defined about the $Rt_{med} \pm FWHM * perfwhm$. For a single sample `xcmsSet` the selection of peaks starts at the most abundant and goes down to the smaller ones. With a multiple sample set the automatic selection uses the most abundant peak as an representative for every feature group, according to the `xcms` grouping. With the `xsAnnotate` sample parameter a sample selection can be defined to use only specific samples. See [xsAnnotate-class](#) for further information. The FWHM (full width at half maximum) of a peak is estimated as $FWHM = SD * 2.35$. For the calculation of the SD, the peak is assumed as normal distributed.

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 specific 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.

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](#),

plotPsSpectrum-methods

Plot a Pseudospectrum

Description

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

Arguments

object	the <code>xsAnnotate</code> object
pspec	ID of the pseudospectrum to print
log	Boolean, whether the <code>log(intensity)</code> 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 <code>pspec</code> 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](#),

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

<code>object1</code>	a <code>xsAnnotate</code> object with pseudospectra
<code>object2</code>	a <code>xsAnnotate</code> object with pseudospectra
<code>PSpec1</code>	index of pseudospectrum in <code>object1</code>
<code>PSpec2</code>	index of pseudospectrum in <code>object2</code>
<code>method</code>	method to use for distance calculation. See details.
<code>...</code>	<code>mzabs</code> , <code>mzppm</code> 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 all the algorithms which are available is returned by `getOption("BioC")$xcms`. If the nickname of a method is called "meanMZmatch", the help page for that specific method can be accessed with `?specDist.meanMZmatch`.

Value

<code>mzabs</code>	maximum absolute deviation for two matching peaks
<code>mzppm</code>	relative deviations in ppm for two matching peaks
<code>symmetric</code>	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 annotated peak data*

Description

This class transforms a `xcmsSet` object with peaks from multiple LC/MS or GC/MS samples into a set of annotation results. It contains searching algorithms for isotopes and adducts, peak grouping algorithms to find connected peak, which originate from the same molecule.

Objects from the Class

Objects can be created with the `xsAnnotate` constructor which include the peaktable from a provided `xcmsSet`. 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 annotation
`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

xsAnnotate constructor for an provided xcmsSet object

Description

This function deals with the construction of an xsAnnotate object. It extracts the peaktable from a provided xcmsSet, which is used for all further analysis. The xcmsSet can be a single sample or multiple sample experiment. Since some functions needs the raw data a selection algorithm must be chosen in the case of a multiple sample. CAMERA includes two different strategies: A defined selection of samples (sample = indices of samples) or the default automatic solution (sample = NA). The automatic solution chooses the best sample for a specific groups called pseudospectrum, see [groupFWHM](#) and [groupCorr](#). It returns a xsAnnotate object, see [xsAnnotate-class](#).

Usage

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

Arguments

xs	a xcmsSet object
sample	Indices of the group xcmsSet sample, that are used for the EIC correlation step. For automatic selection don't set a value. For use all samples simply define sample = c(1:n), with n = number of samples.
nSlaves	For parallel mode set nSlaves higher than 1, but not higher than the number of cpu cores.

Value

A xsAnnotate object.

Author(s)

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

See Also

[xsAnnotate-class](#)

Examples

```
library(faahKO)
xs <- group(faahko)
xsa <- xsAnnotate(xs, sample=c(1:12))

#With automatic selection
xsa.autoselect <- xsAnnotate(xs)
```

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