CAMERA

April 19, 2010

`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(xs, sigma = 6, perfwhm = 0.6, cor_eic_th = 0.75, maxcharge = 3, maxiso
```

Arguments

`xs`	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
`category`	Which class label should be used
`polarity`	Which polarity mode was used for measuring of the ms sample

Details

Batch script for a annotation for a a (grouped) xcmsSet `xs`. Generate intern a xsAnnotate object and calls the member function for the annotation step. Returns a peaklist with additonal columns for isotopes, adducts and an index for the pseudo spectra group. xsAnnotate groups Peaks into spectra groups, after there Retentiontime and EIC correlations. Attention: For the EIC correlation only one sample can be used, so if the xcmsSet contains more than one sample, one must be chosen.

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))
annotated_xs<- annotate(xs)
```

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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

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 <- groupCorr(an,xs) # optional but very recommended step

an <- findIsotopes(an)  # optional but recommended.
an <- findAdducts(an,polarity="positive")
peaklist <- getPeaklist(an) # get the annotated peak list
```

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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 and groupCorr. Generates a list of all possible isotopes, which is stored in object@isotopes.

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)
```

getPeaklist *Retrieve the annotatad peaklist*

Description

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

Usage

```
getPeaklist(object)
```

Arguments

object	xsAnnotate object

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.

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)
  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)
```

Arguments

`object`	the `xsAnnotate` object
`cor_eic_th`	correlation threshold for the EIC correlation

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.

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)
an   <- groupCorr(an)
```

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

Description

Grouping the peaks after the FWHM of the retentiontimes into pseudospectragroups for a xsAnnotate object. 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

The FWHM (full width at half maximum) of a peak, will be used for the grouping. 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. FWHM is calculated as the product of sigma * standard deviation.

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)
```

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, pspecIdx=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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plotPeaks-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
sleep	Time (in seconds) to wait between successive Spectra, if multiple pspec are requested.

Value

None.

Methods

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

Author(s)

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

See Also

`xsAnnotate-class`, `png`, `pdf`, `postscript`,

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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.

`category`: A single string category

`grp_info`: grp_info

`isoID`: isoID

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

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

`xcmsSet`: The embedded xcmsSet, from which the annotation was created

`peaks`: matrix containing peak data

`pspectra`: list containing peak data

`isotopes`: matrix containing peak data

`derivativeIons`: matrix containing peak data

`formula`: matrix containing peak data

`sample`: the number of the used xcmsSet sample

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 EIC

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 is generate from a xcmsSet object adapt its peaktable.

Usage

```
xsAnnotate(xs = NULL,sample=NA,category=NA)
```

Arguments

`xs`	a `xcmsSet` object
`sample`	Index of the group xcmsSet sample, that is used for the EIC corelations step.
`category`	Class label, for the class label of a grouped xcmsSet with different classes.

Value

A `xsAnnotate` object.

Author(s)

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

See Also

xsAnnotate-class

Examples

```
library(faahKO)
xs <- group(faahko)
xs_anno <- xsAnnotate(xs, sample=1, category="WT")
```

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