Package ‘CAMERA’

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Author Carsten Kuhl, Ralf Tautenhahn, Hendrik Treutler, Steffen Neumann {ck-uhlhl|treutle|sneumann}@ipb-halle.de, rtautenh@scripps.edu
Maintainer Steffen Neumann <sneumann@ipb-halle.de>
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### annotate-methods

**Description**

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

**Usage**

```r
annotate(object, sample=NA, nSlaves=1, sigma=6, perfwhm=0.6, 
cor_eic_th=0.75, graphMethod="hcs", pval=0.05, calcCaS=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

```r
library(CAMERA)
file <- system.file("/quotesingle.Varmzdata/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

```r
annotateDiffreport(object, sample=NA, nSlaves=1, sigma=6, perfwhm=0.6, 
cor_eic_th=0.75, cor_exp_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 for EIC correlation (0..1)
- `cor_exp_th`: groupCorr: Threshold for intensity correlations across samples (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
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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)
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 intensites 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

```r
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)
```

**Description**

Processing an xsAnnotate object and correlates peak EIC curves from one pseudospectrum, using a precalculated EIC matrix (`getAllPeakEICs`). It returns 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**

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

**Arguments**

- `object`: The xsAnnotate object
- `EIC`: EIC Matrix
- `corval`: Correlation threshold for the EIC correlation
- `pval`: p-value for testing correlation of significance
- `psg_list`: Vector of pseudospectra indices. The correlation analysis will only be done for those groups

**Details**

The algorithm correlates the EIC of every peak with all others, to find the peaks that belong to one substance. LC/MS data should be grouped with `groupFWHM` first. This step reduces the runtime a lot and increases 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`
**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**

- calcCaS
- groupCorr
- getAllPeakEICs
- xsAnnotate-class
- calcPC
- xsAnnotate-class
Description

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

Usage

calcPC(object, method, ...)

Arguments

- **object**: xsAnnotate-class object
- **method**: Method to use for clustering. See details.
- **...**: 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 nicknames 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

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.hcs(object, ajc=NULL, psg_list=NULL)
```

Author(s)
Carsten Kuhl, <ckuhl@ipb-halle.de>

See Also
calcPC groupCorr highlyConnSG xsAnnotate-class

calcPC.lpc

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

cleanParallel  Cleans up with spawned slave processes after use

Description

The spawned slaves processes, which are created within the parallel mode, are closed explicit.

Usage

cleanParallel(object)

Arguments

object  xsAnnotate object

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

```r
## Not run: library(CAMERA)
file <- system.file("/mzdata/MM14.mzdata", package = "CAMERA")
x <- xcmsSet(file, method="centWave", ppm=30, peakwidth=c(5,10))
an <- xsAnnotate(xs, polarity="positive", nSlaves=2)
an <- groupFWHM(an)
an <- findAdducts(an)
cleanParallel(an)
## End(Not run)
```
compoundLibraries

Author(s)

Carsten Kuhl <ckuhl@ipb-halle.de>

Examples

```r
## Not run:
# Searches for M+H/M-H combinations within a retention time window of 2 seconds
peaklist.pos <- combinexsAnnos(xsa.pos, xsa.neg, tol=2)
## End(Not run)
```

compoundLibraries

The supported compound databases

Description

Returns a set of supported compound databases

Usage

```r
compoundLibraries()
```

Value

Vector of supported compound databases

Author(s)

Hendrik Treutler

Examples

```r
compoundLibraries()
```

compoundQuantiles

compoundQuantiles constructor

Description

constructor of class compoundQuantiles

Usage

```r
compoundQuantiles(compoundLibrary = "kegg", massWindowSize = 50)
```

Arguments

- `compoundLibrary` 
  the database; see `compoundLibraries()` for a list of supported databases
- `massWindowSize` 
  the mass window size for grouping compounds; see `massWindowSizes(compoundLibrary = "kegg")` for a list of supported databases for e.g. the database kegg
compoundQuantiles-class

Value

the compoundQuantiles object

Author(s)

Hendrik Treutler

Examples

cpObj <- compoundQuantiles()

Description

The user is able to get the expected number of atoms of element e (C, N, ...) for a compound of mass m for a q-quantile. I.e. getAtomCount(object = compoundQuantiles(), element = e, mass = m, quantile = q) returns the number of atoms of element e in a compound of mass m in the lowest-(q*100) (sorted ascending by the possible number of atoms of element e for compounds of such mass).

The user is able to get the expected proportion between the intensities of two isotope peaks for a compound of mass m for a q-quantile. I.e. getIsotopeProportion(object = compoundQuantiles(), isotope1 = i1, isotope2 = i2, mass = m, quantile = q) returns the isotope proportion i1 / i2 for a compound of mass m in the lowest-(q*100) (sorted ascending by the possible isotope proportions for compounds of such mass).

Objects from the Class

Objects can be created with the compoundQuantiles constructor.

Slots

compoundLibrary: The compound library to rely on (kegg, chebi, ...)
massWindowSize: The mass window size of the compound statistics (25, 100, ...)
minCompoundMass: Minimum compound mass for which there are statistics
maxCompoundMass: Maximum compound mass for which there are statistics
numberOfMassWindows: Number of mass windows
numberOfIsotopes: Number of isotopes for which there are isotope ratio quantiles
isotopeSet: The set of isotopes for which there are isotope ratio quantiles
elementSet: The set of elements for which there are element count statistics
quantileSet: The set of quantiles for which there are isotope ratio statistics
eleCounters_e_q_mw: Three dimensional array containing the element count statistics (element, quantile, mass window index)
proportions_i_q_mw: Three dimensional array containing the isotope ratio quantiles relative to the monoisotopic peak (isotope index, quantile, mass window index)
findAdducts-methods

Methods

**getAtomCount** signature(object = "xsAnnotate"): returns the number of atoms of the specified element for the given quantile and mass window index

**getIsotopeProportion,compoundQuantiles-method** signature(object = "xsAnnotate"): returns the isotope ratio of the specified isotope for the given quantile and mass window index relative to the monoisotopic peak

Note

No notes yet.

Author(s)

Hendrik Treutler, <hendrik.treutler@ipb-halle.de>

See Also

compoundQuantiles getAtomCount getIsotopeProportion

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

```r
findAdducts(object, ppm=5, mzabs=0.015, multiplier=3, polarity=NULL, rules=NULL, max_peaks=100, psg_list=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 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 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  
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=c("maxo","into","intb"), minfrac=0.5, isotopeMatrix = NULL, filter = TRUE)

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
intval       choose intensity values for C12/C13 check. Allowed values are into, maxo, intb
minfrac      in case of multiple samples, percentaged value of samples, which have to contain the correct C12/C13 ratio and are not NA
isotopeMatrix four column m/z-diff and ratio Matrix, for matching isotopic peaks.
filter       Should C12/C13 filter be applied
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 percentaged 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

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

findIsotopesWithValidation

Deconvolute/Annotate LC/ESI-MS data

Description

Annotate validated isotope clusters for a xsAnnotate object. Returns a xsAnnotate object with annotated isotopes. Validation of isotope clusters is based on statistics of the KEGG database implemented in S4 class object compoundQuantiles.

Usage

```r
findIsotopesWithValidation(object, maxcharge=3, ppm=5, mzabs=0.01, intval=c("maxo","into","intb"), validateIsotopePatterns = TRUE, database="kegg")
```

Arguments

- **object**: the xsAnnotate object
- **maxcharge**: max. number of the isotope charge
- **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
- **validateIsotopePatterns**: logical, if TRUE putative isotope clusters are validated based on KEGG database statistics.
- **database**: the database which is the basis for isotope cluster validation. One of compoundLibraries().
Details

Isotope peaks are annotated for a `xsAnnotate` object according to given rules (maxcharge, maxiso). The algorithm benefits from an 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 ratios between isotope peaks are checked against the mass-specific 99% confidence interval based on statistics of the KEGG database.

Author(s)

Hendrik Treutler <hendrik.treutler@ipb-halle.de>

References

Hendrik Treutler and Steffen Neumann. "Prediction, detection, and validation of isotope clusters in mass spectrometry data". Submitted to Metabolites 2016, Special Issue "Bioinformatics and Data Analysis".

See Also

`findIsotopes`

Examples

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

---

**findKendrickMasses**

Find specific mass defects using Kendrick mass scales

Description

Todo

Usage

```r
findKendrickMasses(object, masses=c(14, 14.01565),
                   maxHomologue=4, error=0.002, time=60, intval="maxo",
                   plot=FALSE)
```

Arguments

- **object**: `xsAnnotate` object
- **masses**: nominal mass and exact mass
- **error**: allowed mass difference in Da for matching Kendrick mass defect
- **maxHomologue**: max number of homologue
- **time**: allowed retention time difference between homologues
- **intval**: intensity value (allowed values: maxo, into or intb)
- **plot**: plot hits
Author(s)

Carsten Kuhl <ckuhl@ipb-halle.de>

Examples

library(CAMERA)
library(faahKO)
xs <- group(faahko)

#With specific selected sample
xsa <- xsAnnotate(xs)

#Screen for substance with CH2 differences
findKendrickMasses(xsa, masses=c(14, 14.01565), plot=TRUE)

---

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 an 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**

```r
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**

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

---

getAllPeakEICs  
**Generate EIC information from raw data**

**Description**

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

**Usage**

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

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)
x.sgrp <- group(faahko)

#create xsAnnotate object
xsa <- xsAnnotate(x.sgrp)
#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;
The number of atoms of the given element

Description

Returns the number of atoms the specified element in a compound of the specified mass for the specified quantile level

Usage

## S4 method for signature 'compoundQuantiles'
getAtomCount(object, element, mass, quantile)

Arguments

object A compoundQuantiles object
element The element of interest specified by element symbol
mass The mass of the compound specified in atomic units (=dalton)
quantile The quantile level for the number of atoms

Value

The number of atoms

Author(s)

Hendrik Treutler

Examples

cpObj <- compoundQuantiles()

compoundMass <- 503
quantileLow <- 0.05
quantileHigh <- 0.95
element <- "C"
countLow <- getAtomCount(object = cpObj, element = element, mass = compoundMass, quantile = quantileLow)
countHigh <- getAtomCount(object = cpObj, element = element, mass = compoundMass, quantile = quantileHigh)

print(paste("The ",(quantileHigh - quantileLow) * 100,"% confidence interval for the number of atoms of element ",element," is ",countLow," and ",countHigh," \)"))
getIsotopeCluster

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 m\textsubscript{z} and intensity value.

Usage

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

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
sampleIndex Selection vector with indexes to select from which sample(s) the intensity values should be retrieved. If set to NULL the sample is selected, which has been chosen for the pseudospectra in the grouping step

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.

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)
getIsotopeProportion, compoundQuantiles-method

The proportion of the intensities of two isotope peaks

**Description**

Returns the proportion of the intensities of isotope1 versus isotope2 for a compound of the given mass for the given quantile level

**Usage**

```r
## S4 method for signature 'compoundQuantiles'
getIsotopeProportion(object, isotope1, isotope2, mass, quantile)
```

**Arguments**

- **object**: A `compoundQuantiles` object
- **isotope1**: The divident isotope ranging from 0 (the monoisotopic peak) to 5
- **isotope2**: The divisor isotope ranging from 0 (the monoisotopic peak) to 5
- **mass**: The mass of the compound specified in atomic units (=dalton)
- **quantile**: The quantile level for the isotope proportion

**Value**

The isotope proportion

**Author(s)**

Hendrik Treutler

**Examples**

```r
cpObj <- compoundQuantiles(compoundLibrary = "kegg")
compoundMass <- 503
isotope1 <- 0
isotope2 <- 1
quantileLow <- 0.05
```
quantileHigh <- 0.95

propLow <- getIsotopeProportion(object = cpObj, isotope1 = isotope1, isotope2 = isotope2, mass = compoundMass, quantile = quantileLow)
propHigh <- getIsotopeProportion(object = cpObj, isotope1 = isotope1, isotope2 = isotope2, mass = compoundMass, quantile = quantileHigh)
print(paste("The ", (quantileHigh - quantileLow) * 100, ",% confidence interval for the proportion of isotopes ", isotope1, " / ", isotope2, " in a compound with mass ", compoundMass, " is [", propLow, ", ", propHigh, "]", sep = ""))

---

getPeaklist

*Generate the annotated peaklist*

**Description**

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

**Usage**

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

**Arguments**

- `object`: xsAnnotate object
- `intval`: Choose intensity values. Allowed values are into, maxo, intb

**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**

```r
library(CAMERA)
file <- system.file("/quotesingle.Varmzdata/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 their EIC correlation and FWHM. These function extract one or more of these so called "pseudo spectra groups" with include the peaklist with their 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",
          calcCiso = FALSE, calcCiS = TRUE, calcCaS = FALSE, psg_list=NULL, xraw=NULL,
          cor_exp_th=0.75, ...)

...
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 information for graph clustering

- **calcCiS**
  - Calculate correlation inside samples

- **calcCaS**
  - Calculate correlation across samples

- **psg_list**
  - Vector of pseudospectra indices. The correlation analysis will be only done for those groups

- **xraw**
  - Optional xcmsRaw object, which should be used for raw data extraction

- **cor_exp_th**
  - Threshold for intensity correlations across samples

- **...**
  - 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 information 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

```r
library(CAMERA)
file <- system.file('mzdata/MM14.mzdata', package = "CAMERA");
x <- xcmsSet(file, method="centWave", ppm=30, peakwidth=c(5, 10));
an <- xsAnnotate(x);
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
xs <- xsAnnotate(xs.grp, sample=1)
```
groupDen

Density-Grouping of LC/ESI-MS data

Description

Group peaks of a xsAnnotate object according to peak distributions in chromatographic time into pseudospectra-groups. Works analogous as the group.density method of xcms. Returns xsAnnotate object with pseudospectra informations.

Usage

`groupDen(object, bw = 5 , ...)`

Arguments

- `object` the xsAnnotate object
- `bw` bandwidth (standard deviation or half width at half maximum) of gaussian smoothing kernel to apply to the peak density chromatogram
- `...` Further Arguments, NYI

Details

The grouping strongly depends on the bw parameter. For an UPLC a good starting point is smaller or around 1.

Value

Returns a grouped xsAnnotate object.

Author(s)

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

```r
library(CAMERA)
# Single sample
file <- system.file('mzdata/MM14.mzdata', package = "CAMERA")
xs <- xcmsSet(file, method="centWave", ppm=30, peakwidth=c(5,10))
xs.grp <- groupDen(xs, bw=0.5)

# Multiple sample
library(faahKO)
xs <- group(faahKO)

# With specific selected sample
xsa <- xsAnnotate(xs, sample=1)
xsa.grp <- groupDen(xsa)

# With automatic selection
xsa.auto <- xsAnnotate(xs)
xsa.grp.auto <- groupDen(xsa.auto)
```

---

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

### Description

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

### Usage

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

### Arguments

- **object**: the xsAnnotate object  
- **sigma**: the multiplier of the standard deviation  
- **perfwhm**: percentage of the width of the FWHM  
- **intval**: intensity values for ordering. Allowed values are into, maxo, intb

### 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 +/- 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](https://github.com/Example/Example) 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.
massWindowSizes

Author(s)

Carsten Kuhl <ckuhl@ipb-halle.de>

Examples

library(CAMERA)
#Single sample
file <- system.file("/quotesingle.Varmzdata/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)
x <- 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)
x.group.auto <- groupFWHM(xs.anno.auto)

massWindowSizes The supported mass window sizes

Description

Returns the set of supported mass window sizes for the given compound database

Usage

massWindowSizes(libraryName = "kegg")

Arguments

libraryName The compound database

Value

Vector of supported mass window sizes

Author(s)

Hendrik Treutler

Examples

massWindowSizes()
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

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 xsAnnotate
- **maxlabel**: How many m/z labels to print
- **sleep**: seconds to pause between plotting EICs
- **...**: other graphical parameters

Value
None.

Methods

```r
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.

Usage

```r
plotPsSpectrum(object, pspec=1:length(object$pspectra), log=FALSE, value="into", maxlabel=0, ti
```
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.
cexMulti  Cex multiplier for peak labels
...  Additional parameter for function plot

Value

None.

Methods

signature(object = "xsAnnotate") object deriviving from class "xsAnnotate"

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

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, nzppm 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")$xcms$specDist.methods.

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 Kutzer, <jkutzer@ipb-halle.de>

pspec2metfrag

Export the putative fragments as MetFrag query files

Description

MetFrag is an in-silico metabolite identification system, which aims to putatively identify compounds from fragmentation MS data, especially from tandem-MS, but also in-source fragments might give additional hints on top of the accurate mass of the precursor alone.

Usage

pspec2metfrag(object, pspecidx=NULL, filedir=NULL)
ppec2metfusion(object, pspecidx=NULL, filedir=NULL)

Arguments

- object: an xsAnnotate object
- pspecidx: Index of pspectra to export, if NULL then all are exported.
- filedir: Directory for placement of batch query files

Details

For each spectrum in pspecidx (or all in the xsAnnotate object), for each [M] mass hypothesis, remove all non-fragment peaks (isotopes, clusters, adducts) and pass them to MetFrag and MetFusion batch query files.
Value

Returns a list

Author(s)

Carsten Kuhl <ckuhl@ipb-halle.de>

Examples

```r
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 step
an <- findAdducts(an, polarity="positive")
pspec2metfrag(an, pspecidx=c(1))
```

ruleSet

Class ruleSet

Description

The class ruleSet is used to read lists of ions, adducts and neutral losses, and compile the dynamic ruleSet from those. This makes it possible to modify the default rules for certain analytical settings.

Slots

- ionlistfile: File of known charged ions, an example is found in CAMERA/lists/ions.csv.
- neutrallossfile: File of known neutral losses, an example is found in CAMERA/lists/neutralloss.csv.
- neutraladditionfile: File of known adducts, an example is found in CAMERA/lists/lists/neutraladdition.csv.
- ionlist: Known charged ions.
- neutralloss: Known neutral losses.
- neutraladdition: Known adducts.
- maxcharge:.
- mol:.
- nion:.
- nnloss:.
- nnadd:.
- nh:.
- polarity: Polarity of the ruleSet.
- rules: data.frame of resulting mass differences, this is the dynamic ruleSet.
- lib.loc Path to local R library
Extends

Class "Versioned", directly.

Methods

Methods implemented for ruleSet

setDefaultLists signature(object = "ruleSet"): Set filenames for the lists shipped with CAMERA.

readLists signature(object = "ruleSet"): Read and parse the lists from the files.

setDefaultParams signature(object = "ruleSet"): Set the default parameters for rule generation.

setParams signature(object = "ruleSet"): Set the parameters for rule generation.

generateRules signature(object = "ruleSet"): Create the rules in ruleSet@rules.

Author(s)

Steffen Neumann and Carsten Kuhl

Examples

```
r <- new("ruleSet");
r2 <- setDefaultLists(r);
r3 <- readLists(r2);
r4 <- setDefaultParams(r3);
r5 <- generateRules(r4);
dim(r5@rules)
```

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 choosen 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, polarity = NULL)
```
**xsAnnotate-class**

**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.
- **polarity**: Set polarity mode: "positive" or "negative"

**Value**

A `xsAnnotate` object.

**Author(s)**

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

**See Also**

`xsAnnotate-class`

**Examples**

```r
library(faahKO)
xs <- group(faahKO)
xsA <- xsAnnotate(xs, sample=c(1:12))
#With automatic selection
xsA.autoselect <- xsAnnotate(xs)
```

**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 assignment 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) Peaktetable with "into" values
- `isotopes`: List with annotated isotopic 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`
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