Package ‘CAMERA’

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Description Annotation of peaklists generated by xcms, rule based annotation of isotopes and adducts, isotope validation, EIC correlation based tagging of unknown adducts and fragments
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annotate-methods

Automatic deconvolution/annotation of LC/ESI-MS data

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, 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] clustersions
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>
Experiments

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
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, calcC1S=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
calcC1S 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
annotateDiffreport

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 speed up 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 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 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
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
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 algorithm clusters peaks from a xsAnnotate object into pseudospectra according to a provided distance matrix. Therefore all peaks are transformed 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.

gitoPTION("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

Peakclustering into pseudospectra with the highly connected subgraphs approach

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

Peakclustering into pseudospectra with the label-propagation-community algorithm

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("/quotesingle.Var
mzdata/MM14.mzdata", package = "CAMERA")
xs <- 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)
```

combinexsAnnos

Check CAMERA ion species annotation due to matching with opposite ion mode

Description

This function check annotations of ion species with the help of a sample from opposite ion mode. As first step it searches for pseudospectra from the positive and the negative sample within a retention time window. For every result the m/z differences between both samples are matched against specific rules, which are combinations from pos. and neg. ion species. As example M+H and M-H with a m/z difference of 2.014552. If two ions matches such a difference, the ion annotations are changed (previous annotation is wrong), confirmed or added. Returns the peaklist from one ion mode with recalculated annotations.

Usage

```r
combinexsAnnos(xsa.pos, xsa.neg, pos=TRUE, tol=2, ruleset=NULL)
```

Arguments

- `xsa.pos`: xsAnnotate object with positive ion mode
- `xsa.neg`: xsAnnotate object with negative ion mode
- `pos`: If TRUE the peaklist from the positive mode is returned, if FALSE the negative
- `tol`: Retention time window in seconds
- `ruleset`: Matrix of matching rules, see example

Details

Both xsAnnotate object should be full processed (grouping and annotation). Without previous annotation the resulting peaklist only includes annotation with matches peaks from both mode according to the rule(s). With ruleset=NULL the function only looks for M+H/M-H pairs. The ruleset is a two column matrix with includes rule indices from the rule table of both xsAnnotate objects. ruleset <- cbind(1,1) would create the M+H/M-H rule, since the first rule of xsa.pos@ruleset and xsa.neg@ruleset is M+H respectively M-H. Only rules with identical charge can be combined!

Value

Returns a (normal) CAMERA peaklist with a additional column neg. Mode or pos. Mode, where matching peaks from the opposite mode are noted.
compoundLibraries

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

Examples

## 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
compoundLibraries()

Value
Vector of supported compound databases

Author(s)
Hendrik Treutler

Examples

compoundLibraries()

compoundQuantiles

compoundQuantiles constructor

Description
constructor of class compoundQuantiles

Usage
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()

compoundQuantiles-class

Class compoundQuantiles encapsulates compound statistics from different databases.

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)
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
findAdducts(object, ppm=5, mzabs=0.015, multiplier=3, polarity=NULL, rules=NULL, max_peaks=100, psg_list=NULL, intval="maxo")

Arguments

<table>
<thead>
<tr>
<th>Argument</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>object</td>
<td>the xsAnnotate object</td>
</tr>
<tr>
<td>ppm</td>
<td>ppm error for the search</td>
</tr>
<tr>
<td>mzabs</td>
<td>allowed variance for the search</td>
</tr>
<tr>
<td>multiplier</td>
<td>highest number(n) of allowed clusterion [nM+ion]</td>
</tr>
<tr>
<td>polarity</td>
<td>Which polarity mode was used for measuring of the ms sample</td>
</tr>
<tr>
<td>rules</td>
<td>personal ruleset or with NULL standard ruleset will be calculated</td>
</tr>
<tr>
<td>max_peaks</td>
<td>If run in parralel mode, this number defines how much peaks will be calculated in every thread</td>
</tr>
<tr>
<td>psg_list</td>
<td>Vector of pseudospectra indices. The correlation analysis will be only done for those groups</td>
</tr>
<tr>
<td>intval</td>
<td>choose intensity values. Allowed values are into, maxo, intb</td>
</tr>
</tbody>
</table>
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 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
findIsotopesWithValidation

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 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
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
findIsotopesWithValidation(object, maxcharge=3, ppm=5, mzabs=0.01, intval=c("maxo","into","intb")

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 $\pm 99\%$ 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
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 <- findIsotopesWithValidation(an)

findKendrickMasses

Description
Find specific mass defects using Kendrick mass scales

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

Arguments

<table>
<thead>
<tr>
<th>Argument</th>
<th>Description</th>
</tr>
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</table>
findNeutralLoss

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)
xp.spseudo@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 Pseudspecta with water loss
hits <- findNeutralLossSpecs(an, mzdiff=18.01, mzabs=0.01)

generatePeakEICs  
Generate EIC information from raw data

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

Usage
generatePeakEICs(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)
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;
getAtomCount,compoundQuantiles-method

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

```r
## 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

```r
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 ",
```
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", 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("/quotesingle/var/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)
# Select from multiple samples

```r
isolist <- getIsotopeCluster(an, sampleIndex=c(1,2,5))
```

## Interaction with Rdisop

```r
## 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)
```

---

**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 \[", propLow, ", \", propHigh, ",\]"))

---

**getPeaklist**

*Generate the annotated peaklist*

**Description**

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

**Usage**

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

**Arguments**

- **object**: xsAnnotate object
- **intval**: Choose intensity values. Allowed values are into, maxo, intb, intf, maxf, area, depending on the feature detection algorithm used.

**Details**

This function extracts 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('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 the EIC correlation and FWHM. These functions 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))

getReducedPeaklist  
Generate reduced peaklist from the annotated peaklist

Description
Extract information from an xsAnnotate object. Returns a reduced peaklist with annotated peaks. For any putative compound in the pcgroup, all found adducts are pooled into one putative compound per group. Thus, the reduced peaklist only contains one annotated adduct per pcgroup.

Usage
getReducedPeaklist(object, method = "median", intval = "into", default.adduct.info = "first", mzrt.range = FALSE, npeaks.sum = FALSE, cleanup = FALSE)
getReducedPeaklist

Arguments

object xsAnnotate object.
method Choose reduction method. Allowed values are "sum", "median", "maxint", "pca".
intval Choose intensity values. Allowed values are "into", "maxo", "intb".
default.adduct.info Choose method to select adduct information. Allowed values are "first", "max-int", "maxpeaks"
mzrt.range If TRUE, max and min values of mz and rt values of all adducts within a pc-group are saved (not recommended).
npeaks.sum If TRUE, the sum of all peaks of all adducts within a pcgroup is saved (not recommended).
cleanup If TRUE, NA values and negative abundances are being set to zero and constant features (rows) are being removed.

Details

This function extracts a reduced peaktable from an xsAnnotate object. Normally, all adducts are grouped for any putative compounds and saved within the peaklist (see method getPeaklist). However, for statistical computation it is sometimes better to only work with putative compounds rather than with all of their adducts. Thus, this function pools all adducts for any putative compound into one putative compound per pcgroup. There are several methods to choose from how this is being done. Selection methods: "sum": The intensities of adducts are summed for each sample. "median" (default): The median intensities of adducts is calculated for each sample. "maxint": Only the adduct with the highest intensities throughout the samples is returned. "pca": A Principal Component Analysis is being performed for the adducts for the samples. and the PC1 values are taken as intensity information. Select mz / rt methods: "first" (default): The mz & rt information of the first adduct are taken. "maxint": The mz & rt information of the adduct that has highest intensities are taken. "maxpeaks": The mz & rt information of the adduct that has the most peaks are taken. In addition, when mzrt.range is TRUE, the min and max values of all mz and rt found in a group are stored within mzmin, mzmax and rtmin and rtmax (not recommended). In addition, when npeaks.sum is TRUE, all peaks within a pcgroup are summed (not recommended).

Author(s)

Kristian Peters <kpeters@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.reduced <- getReducedPeaklist(an)
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

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

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
- **xraw**: Optional xcmsRaw object, which should be used for raw data extraction
- **cor_exp_th**: Threshold for intensity correlations across samples
- **intval**: Selection of the intensity values (such as "into") that should be used in the correlation analysis. See `getPeaklist` for all allowed values.
- **...**: Additional parameter

Details

The algorithm calculates different informations for group peaks into so called pseudospectra. This pseudospectra contains peaks, with 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 informations 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("/Var\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(xs.grp)
xsa.grp <- groupFWHM(xsa.auto)
xsa.iso <- findIsotopes(xsa.grp) #optional step
index <- c(1,4) #Only group one and four will be calculate
#We use also correlation across sample
xsa.grp.corr <- groupCorr(xsa.iso, psu_list=index, calcIso=TRUE, calcCaS=TRUE)
#Note: Group 1 and 4 have no subgroups
```

---

**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("/quotesingle.varmzdata/MM14.mzdata", package = "CAMERA")
xs <- xcmsSet(file, method="centWave", ppm=30, peakwidth=c(5,10))
xsa <- xsAnnotate(xs)
xsa.grp <- groupDen(xsa, 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)
```

Description

FWHM-Grouping of LC/ESI-MS data

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
massWindowSizes

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 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")
x <- xcmsSet(file, method="centWave", ppm=30, peakwidth=c(5,10))
an <- xsAnnotate(x)
an <- groupFWHM(an)

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

#With specific selected sample
xs.anno <- xsAnnotate(xs, sample=1)
x.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
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>
plotEICs-methods

Source


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 `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, title=NULL, mzrange=numeric(), sleep=0, cexMulti = 1, ...)
```

**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**

```r
signature(object = "xsAnnotate") object deriving from class "xsAnnotate"
```

**Author(s)**

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

**See Also**

- `xsAnnotate-class.png.pdf.postscript`
**psDist-methods**

**Distance methods for xsAnnotate**

**Description**

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

**Arguments**

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

**Details**

Different algorithms can be used by specifying them with the `method` argument. For example to use the "meanMZmatch" approach one would use: `specDist(object1, object2, psppectrum1, 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, psppectrum1, 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)
pspec2metfusion(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)

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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 <- groupPWHM(an);
an <- findIsotopes(an); #optional step
an <- findAdducts(an, polarity="positive")

pspec2metfrag(an, pspecidx=c(1))
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
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 need 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 group called pseudospectrum, see groupFWHM and groupCorr. It returns a xsAnnotate object, see xsAnnotate-class.

Usage

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

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)

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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)
```

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 peaktab 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) Peaktab 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.

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See Also

xsAnnotate
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