Package ‘CAMERA’
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annotate-methods

Automatic deconvolution/annotation of LC/ESI-MS data

Description

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

Usage

annotate(object, sample=NA, nSlaves=1, sigma=6, perfwhm=0.6, cor_eic_th=0.75, graphMethod="hcs", pval=0.05, calcCiS=TRUE, calcIs=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  
 sample  
 nSlaves  
 sigma  
 perfwhm  
 cor_eic_th  
 graphMethod  
 pval  
 calcCiS  
 calcIso  
 calcCaS  
 maxcharge  
 maxiso  
 minfrac  
 ppm  
 mzabs  
 quick  
 psg_list  
 rules  
 polarity  
 multiplier  
 max_peaks  
 intval

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

---

**annotateDiffreport**  
*Automatic deconvo/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
annotateDiffreport

psg_list Calculation will only be done for the selected groups
diffAdducts: 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)
x.s.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

```r
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)
x_s.grp <- group(faahko)
# create xsAnnotate object
xsa <- xsAnnotate(x_s.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`: pvalue for testing correlation of significance
- `psg_list`: Vector of pseudospectra indices. The correlation analysis will be only done for those groups

Details

The algorithm correlates the EIC of 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:

<table>
<thead>
<tr>
<th>column</th>
<th>description</th>
</tr>
</thead>
<tbody>
<tr>
<td>x</td>
<td>peak index</td>
</tr>
<tr>
<td>y</td>
<td>peak index</td>
</tr>
<tr>
<td>cor</td>
<td>edge value, always 1</td>
</tr>
<tr>
<td>ps</td>
<td>pseudospectrum index, which contains x and y</td>
</tr>
</tbody>
</table>

Methods

object = "xsAnnotate" calcIsotopes(object)

Author(s)

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

See Also

calcPC xsAnnotate-class
calcPC-methods

Peakclustering into pseudospectra according to a distance matrix

Description

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

Usage

calcPC(object, method, ...)

Arguments

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.

ggetOption("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 retention time 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**

```r
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
cleanParallel

Arguments

object   xsAnnotate object
aje   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 sepa-
ration. 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>
combinexsAnnos

## Not run
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, polarity="positive", nSlaves=2)
am <- 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 annotation 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

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
		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
```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)
```

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
```r
compoundLibraries()
```

compoundQuantiles

compoundQuantiles constructor

Description
constructor of class compoundQuantiles

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

Arguments
```r
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
```
The compoundQuantiles object

Author(s)

Hendrik Treutler

Examples

```r
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

```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
findIsotopes

Deconvolute/Annotate LC/ESI-MS data

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

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

Description

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

Usage

```r
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("/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)

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"), 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().
findKendrickMasses

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('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 Find specific mass defects using Kendrick mass scales

Description

Todo

Usage

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
findNeutralLoss

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

Examples

library(CAMERA)
library(faahKO)
xr <- 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 a artificial xcmsSet, where the peaks with the specific neutral loss are stored in xcmsSet@peaks.

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

Examples

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

# Searches for Peaks with water loss
xr.pseudo <- findNeutralLoss(an, mzdiff=18.01, mzabs=0.01)
xr.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('mzdata/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
ggetAllPeakEICs(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**

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

#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 ", element, " is ", countLow, " to ", countHigh, ", respectively.\n"))
```
**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**

\[ \text{getIsotopeCluster}(\text{object, number=NULL, value="maxo", sampleIndex=NULL}) \]

**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**

```r
# single sample
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)
an <- findIsotopes(an)
isolist <- getIsotopeCluster(an)
isolist[[10]] # get IsotopeCluster 10

# multiple sample
library(faahKO)
x <- group(faahko)
x <- fillPeaks(x)
an <- xsAnnotate(x)
an <- groupFWHM(an)
an <- findIsotopes(an)
isolist <- getIsotopeCluster(an)
```
#Select from multiple samples

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

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

### End(Not run)

---

### 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 

---

### 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

**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/var/mzdata/VM14.mzdata’, package = "CAMERA")
xs <- xcmsSet(file, method="centWave", ppm=30, peakwidth=c(5,10))
an <- xsAnnotate(xs)
an <- groupFWHM(an)
an <- findIsotopes(an)
an <- findAdducts(an,polarity="positive")
peaklist <- getPeaklist(an)
```
getpspectra  

Retrieve a peaklist of one or more pseudospectra

Description

Extract group(s) from a xsAnnotate object. Returns a peaklist as matrix with annotated peaks.

Usage

getpspectra(object, grp)

Arguments

object  xsAnnotate object
grp  index of pseudo-spectra-group

Details

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

Author(s)

Carsten Kuhl <ckuhl@ipb-halle.de>

Examples

library(CAMERA)
file <- system.file("mzdata/MM14.mzdata", package = "CAMERA")
xs <- xcmsSet(c(file), method="centWave", ppm=30, peakwidth=c(5,10))
an <- xsAnnotate(xs)
an <- groupFWHM(an)
#For one group
peaklist <- getpspectra(an, 1)
#For two groups
peaklist <- getpspectra(an, c(1,2))


groupCorr  

EIC correlation grouping of LC/ESI-MS data

Description

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

Usage

groupCorr(object, cor_eic_th=0.75, pval=0.05, graphMethod="hcs",
calcIso = FALSE, calcCI = TRUE, calcCS = FALSE, ps_list=NULL, xraw=NULL,
cor_exp_th=0.75, ...)


**groupCorr**

**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("/path/to/Var.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, psg_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**

```r
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

library(CAMERA)
#Single sample
file <- system.file('mzdata/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)

---

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

Description

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

Usage

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 eluates 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.
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

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

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:

```r
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**

plotPsSpectrum-methods

Plot a Pseudospectrum

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

Usage
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 deriving 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, mzppm and parameters for the distance function.
Details

Different algorithms can be used by specifying them with the method argument. For example, to use the "meanMZmatch" approach, one would use:

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

This is also the default.

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

A character vector of nicknames for all the algorithms 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 Kutzera, <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.
**ruleSet**

**Value**

Returns a list

**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); #optional step
an <- findAdducts(an, polarity="positive")
pspec2metfrag(an, pspcidx=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)

xsAnnotate xsAnnotate constructor for an provided xcmsSet object

Description

This function deals with the construction of an xsAnnotate object. It extracts the peaktable from a provided xcmsSet, which is used for all further analysis. The xcmsSet can be a single sample or multiple sample experiment. Since some functions need 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)
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)
xs <- xsAnnotate(xs, sample=c(1:12))

#With automatic selection
xs.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 peaktabe 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) Peetable 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 selected 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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