Package ‘CAMERA’

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Title Collection of annotation related methods for mass spectrometry data

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Depends R (>= 2.1.0), methods, Biobase, xcms (>= 1.13.5)
Imports methods, xcms, RBGL, graph, graphics, grDevices, stats, utils, Hmisc, igraph

Suggests faahKO, RUnit, BiocGenerics

Enhances Rmpi, snow

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

License GPL (>= 2)

ByteCompile TRUE

URL http://msbi.ipb-halle.de/msbi/CAMERA/

BugReports https://github.com/sneumann/CAMERA/issues/new

biocViews MassSpectrometry, Metabolomics

RoxygenNote 5.0.1

NeedsCompilation yes

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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

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

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

Details

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

Value

annotate returns an xsAnnotate object. For more information about the xsAnnotate object see xsAnnotate-class.

Author(s)

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

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

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

Description

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

Usage

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

Arguments

- `object`: xcmsSet with peak group assignments
- `sample`: xsAnnotate: Sample selection for grouped xcmsSet, see xsAnnotate-class
- `nSlaves`: xsAnnotate: Use parallel CAMERA mode, require Rmpi
- `sigma`: groupFWHM: multiplier of the standard deviation
- `perfwhm`: groupFWHM: percentage of FWHM width
- `cor_eic_th`: groupCorr: Correlation threshold for EIC correlation (0..1)
- `cor_exp_th`: groupCorr: Threshold for intensity correlations across samples (0..1)
- `graphMethod`: groupCorr: Method selection for grouping peaks after correlation analysis into pseudospectra
- `pval`: groupCorr: significant correlation threshold
- `calcCiS`: groupCorr: Use correlation inside samples for peak grouping
- `calcIso`: groupCorr: Use isotopic relationship for peak grouping
- `calcCaS`: groupCorr: Use correlation across samples for peak grouping
- `maxcharge`: findIsotopes: max. ion charge
- `maxiso`: findIsotopes: max. number of expected isotopes
- `minfrac`: findIsotopes: The percentage number of samples, which must satisfy the C12/C13 rule for isotope annotation
- `ppm`: General ppm error
- `mzabs`: General absolut error in m/z
- `quick`: Use only groupFWHM and findIsotopes
annotateDiffreport

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>psg_list</td>
<td>Calculation will only be done for the selected groups</td>
</tr>
<tr>
<td>rules</td>
<td>findAdducts: User defined ruleset</td>
</tr>
<tr>
<td>polarity</td>
<td>findAdducts: Which polarity mode was used for measuring of the ms sample</td>
</tr>
<tr>
<td>multiplier</td>
<td>findAdducts: If no ruleset is provided, calculate ruleset with max. number n of ([nM+x]) clusterions</td>
</tr>
<tr>
<td>max_peaks</td>
<td>How much peaks will be calculated in every thread using the parallel mode</td>
</tr>
<tr>
<td>intval</td>
<td>General used intensity value (into, maxo, intb)</td>
</tr>
<tr>
<td>pval_th</td>
<td>pval threshold. Creates a new psg_list. A pseudospectra is selected if it contains peaks, with pval &lt; pval_th</td>
</tr>
<tr>
<td>fc_th</td>
<td>Same as pval. Select those groups with contains peaks with fold-change &gt; fc_th. Pval_th and fc_th can be combined</td>
</tr>
<tr>
<td>sortpval</td>
<td>Sort diffreport after pvalues</td>
</tr>
</tbody>
</table>

... 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, an 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

```r
# 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)
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**: p-value for testing correlation of significance
- **psg_list**: Vector of pseudospectra indices. The correlation analysis will only be done for those groups

Details

The algorithm correlates the EIC of every peak with all others, to find the peaks that belong to one substance. LC/MS data should be grouped with groupFWHM first. This step reduces the runtime a lot and increases the number of correct classifications. Only correlation with a higher value than the correlation threshold and significant p-values will be returned.

Value

A matrix with 4 columns:

- **x**: peak index
- **y**: peak index
- **cor**: correlation value
- **ps**: pseudospectrum index, which contains x and y
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>x</th>
<th>peak index</th>
</tr>
</thead>
<tbody>
<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
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
### 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
```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
**cleanParallel**

**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.Varmzdata/MM14.mzdata", package = "CAMERA")
x <- xcmsSet(file, method="centWave", ppm=30, peakwidth=c(5,10))
an <- xsAnnotate(x, 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 annoations 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**

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

---

**compoundLibraries**  
*The supported compound databases*

**Description**

Returns a set of supported compound databases

**Usage**

```r
compoundLibraries()
```

**Value**

Vector of supported compound databases

**Author(s)**

Hendrik Treutler

**Examples**

```r
compoundLibraries()
```

---

**compoundQuantiles**  
*compoundQuantiles constructor*

**Description**

constructor of class compoundQuantiles

**Usage**

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

**Arguments**

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

Value
the compoundQuantiles object

Author(s)
Hendrik Treutler

Examples
```
cpObj <- compoundQuantiles()
```

Description
The user is able to get the expected number of atoms of element e (C, N, ...) for a compound of mass m for a q-quantile. I.e. `getAtomCount(object = compoundQuantiles(), element = e, mass = m, quantile = q)` returns the number of atoms of element e in a compound of mass m in the lowest \((q \times 100)\) (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 \(i_1 / i_2\) for a compound of mass m in the lowest \((q \times 100)\) (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)

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 parralel 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

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
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 percentage of samples, which must passed the test. If peaks are NA, then this sample is skipped and the ratio is (found correct C12/C13 ratio) / (samples containing C12 and C13 peak).

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

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

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

Description

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

library(CAMERA)
file <- system.file('mzdata/MM14.mzdata', package = 'CAMERA')
x <- xsmsSet(file, method="centWave", ppm=30, peakwidth=c(5,10))
an <- xsmsAnnotate(x)
an <- groupFWHM(an)
an <- findIsotopesWithValidation(an)

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)
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 a artificial xcmsSet, where the peaks with the specific neutral loss are stored in xcmsSet@peaks.

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

Examples
library(CAMERA)
file <- system.file("/mzdata/MM14.mzdata", package = "CAMERA")
xs <- xcmsSet(file, method="centWave", ppm=30, peakwidth=c(5,10))
an <- xsAnnotate(xs)
an <- groupFWHM(an)
#Searches for Peaks with water loss
xs.pseudo <- findNeutralLoss(an,mzdiff=18.01,mzabs=0.01)
xs.pseudo@peaks #show Hits
findNeutralLossSpecs  Find pseudospectra that contains a specific neutral loss

Description
The method searches in every pseudospectra for a distance between two ions matching a provided mass difference. It returns a boolean vector with the length equals to the number of pseudospectra, where a hit is marked with TRUE.

Usage
findNeutralLossSpecs(object, mzdiff=NULL, mzabs=0, mzppm=10)

Arguments
object xsAnnotate object
mzdiff neutral loss in Dalton
mzabs absolut allowed mass difference
mzppm relative allowed mass difference

Details
The function needs a xsAnnotate object after groupCorr or groupFWHM.

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

Examples
library(CAMERA)
file <- system.file("mzdata/MM14.mzdata", package = "CAMERA")
xs <- xcmsSet(file, method="centWave", ppm=30, peakwidth=c(5,10))
an <- xsAnnotate(xs)
an <- groupFWHM(an)
#Searches for 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 C in a compound with mass 503 is [", countLow, ",", countHigh, "]", sep = ""))
```
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("mzdata/MM14.mzdata", package = "CAMERA")
xs <- xcmsSet(file, method="centWave", ppm=30, peakwidth=c(5,10))
an <- xsAnnotate(xs)
an <- groupFWHM(an)
an <- findIsotopes(an)
isolist <- getIsotopeCluster(an)
isolist[[10]] # get IsotopeCluster 10

# multiple sample
library(faahKO)
xs <- group(faahko)
xs <- fillPeaks(xs)
an <- xsAnnotate(xs)
an <- groupFWHM(an)
an <- findIsotopes(an)
isolist <- getIsotopeCluster(an)
getIsotopeProportion, compoundQuantiles-method

The proportion of the intensities of two isotope peaks

Description

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

Usage

## 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

cpObj <- compoundQuantiles(compoundLibrary = "kegg")

compoundMass <- 503
isotope1 <- 0
isotope2 <- 1
quantileLow <- 0.05
getPeaklist

```r
quantileHigh <- 0.95
propLow <- getIsotopeProportion(object = cpObj, isotope1 = isotope1, isotope2 = isotope2, mass = compoundMass, quantile = quantileLow)
propHigh <- getIsotopeProportion(object = cpObj, isotope1 = isotope1, isotope2 = isotope2, mass = compoundMass, quantile = quantileHigh)
print(paste("The ", (quantileHigh - quantileLow) * 100, ", % confidence interval for the proportion of isotopes ", isotope1, ": ", isotope2, ", in a compound with mass ", compoundMass, ", is ", propLow, ", ", propHigh, ",", sep = ""))
```

---

**getPeaklist**

*Generate the annotated peaklist*

**Description**

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

**Usage**

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

**Arguments**

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

**Details**

This function extract the peaktable from an xsAnnotate object, containing three additional columns (isotopes, adducts, pseudospectrum) with represents the annotation results. For a grouped xcmsSet it returns the grouped peaktable.

**Author(s)**

Carsten Kuhl <ckuhl@ipb-halle.de>

**Examples**

```r
library(CAMERA)
file <- system.file("/mzdata/MM14.mzdata", package = "CAMERA")
x <- xcmsSet(file, method="centWave", ppm=30, peakwidth=c(5,10))
an <- xsAnnotate(x)
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))
**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, which have a high correlation between each other. So far three different kind of information are available. Correlation of intensities across samples (need more than 3 samples), EIC correlation between peaks inside a sample and additional the information about recognized isotope cluster can be included. After calculation of all these informations, they are combined as edge value into a graph object. A following graph clustering algorithm separate the peaks (nodes in the graph) into the pseudospectra.

**Author(s)**

Carsten Kuhl <ckuhl@ipb-halle.de>

**See Also**

- `calcCiS`
- `calcCaS`
- `calcPC`
- `xsAnnotate-class`

**Examples**

```r
library(CAMERA)
file <- system.file("/mzdata/MM14.mzdata", package = "CAMERA");
x <- xcmsSet(file, method="centWave", ppm=30, peakwidth=c(5, 10));
an <- xsAnnotate(x);
an.group <- groupFWHM(an);
an.iso <- findIsotopes(an.group); #optional step for using isotope information
an.grp.corr <- groupCorr(an.iso, calcIso=TRUE);

# For csv output
# write.csv(file="peaklist_with_isotopes.csv",getPeaklist(an))

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

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

Density-Grouping of LC/ESI-MS data

Description

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

Usage

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

Arguments

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

Details

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

Value

Returns a grouped xsAnnotate object.

Author(s)

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

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

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

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

# With automatic selection
xsauto <- xsAnnotate(xs)
x.grpauto <- groupDen(xsauto)
```

---

**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**

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

**Arguments**

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

**Details**

Every peak who eluate at the same time-point as a selected peak, will be part of the group. Same time-point is defined about the Rt_med +/- FWHM * perfwhm. For a single sample `xcmsSet` the selection of peaks starts at the most abundant and goes down to the smaller ones. With a multiple sample set the automatic selection uses the most abundant peak as a 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("/Var/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

Author(s)

Hendrik Treutler

Examples

massWindowSizes()
Description

xcmsSet object containing quantitated LC/MS peaks from a marker mixture. The data is a centroided subset from 117-650 m/z and 271-302 seconds with 134 peaks. Positive ionization mode data in mzData file format.

Usage

data(mm14)

Format

The format is:

Formal class 'xcmsSet' [package "xcms"] with 8 slots
  @ peaks : num [1:83, 1:11] 117 117 118 119 136
  ..- attr(*) = 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 deriviving from class "xsAnnotate"

Author(s)

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

See Also

xsAnnotate-class, png, pdf, postscript.

Description

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

Arguments

- **object1**: a xsAnnotate object with pseudospectra
- **object2**: a xsAnnotate object with pseudospectra
- **PSpec1**: index of pseudospectrum in object1
- **PSpec2**: index of pseudospectrum in object2
- **method**: method to use for distance calculation. See details.
- **...**: mzabs, mzppm and parameters for the distance function.
Different algorithms can be used by specifying them with the method argument. For example to use
the "meanMZmatch" approach one would use: specDist(object1, object2, pspectrum1, pspectrum2, method="meanMZmatch")
This is also the default.
Further arguments given by ... are passed through to the function implementing the method.
A character vector of nicknames for all the algorithms which are available is returned by getOption("BioC")$xcms$specDist.methods
If the nickname of a method is called "meanMZmatch", the help page for that specific method can
be accessed with ?specDist.meanMZmatch.

Value
mzabs maximum absolute deviation for two matching peaks
mzppm relative deviations in ppm for two matching peaks
symmetric use symmetric pairwise m/z-matches only, or each match

Methods
object1 = "xsAnnotate" specDist(object1, object2, pspectrum1, pspectrum2, method,...)

Author(s)
Joachim 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 com-
 pounds 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, re-
move all non-fragment peaks (isotopes, clusters, adducts) and pass them to MetFrag and MetFusion
batch query files.
**Value**

Returns a list

**Author(s)**

Carsten Kuhl <ckuhl@ipb-halle.de>

**Examples**

```r
library(CAMERA)
file <- system.file('mzdata/MM14.mzdata', package = "CAMERA");
xs <- xcmsSet(file, method="centWave", ppm=30, peakwidth=c(5, 10));
an <- xsAnnotate(xs);
an <- groupFWHM(an);
an <- findIsotopes(an); #optional step
an <- findAdducts(an, polarity="positive")

pspec2metfrag(an, pspecidx=c(1))
```

---

**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 chosen in the case of a multiple sample. CAMERA includes two different strategies: A defined selection of samples (sample = indices of samples) or the default automatic solution (sample = NA). The automatic solution chooses the best sample for a specific groups called pseudospectrum, see groupFWHM and groupCorr. It returns a xsAnnotate object, see xsAnnotate-class.

Usage

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

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

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

\hrule

xsAnnotate-class Class xsAnnotate, a class for annotated peak data

Description

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

Objects from the Class

Objects can be created with the xsAnnotate constructor which include the peaktable from a provided xcmsSet. Objects can also be created by calls of the form new("xsAnnotate", ...).
Slots

- **annoGrp**: Assignment of mass hypotheses to correlation groups
- **annoID**: The 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) Peaktable with "into" values
- **isotopes**: List with annotated isotopid results for every peak
- **polarity**: A single string with the polarity mode of the peaks
- **pspectra**: List contains all pseudospectra with there peak IDs
- **psSamples**: List containing information with sample was sample was selecteted as representative (automatic selection)
- **ruleset**: A dataframe describing the mass difference rules used for the annotation
- **runParallel**: Flag if CAMERA runs in serial or parallel mode
- **sample**: Number of the used xcmsSet sample (beforehand sample selection)
- **xcmsSet**: The embedded xcmsSet

Methods

- **groupFWHM** signature(object = "xsAnnotate"): group the peak data after the FWHM of the retention time
- **groupCorr** signature(object = "xsAnnotate"): group the peak data after the correlation of the EICs
- **findIsotopes** signature(object = "xsAnnotate"): search for possible isotopes in the spectra
- **findAdducts** signature(object = "xsAnnotate"): search for possible adducts in the spectra
- **plotEICs** signature(object = "xsAnnotate"): plot EICs of pseudospectra

Note

No notes yet.

Author(s)

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

See Also

- **xsAnnotate**
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