# Package 'CAMERA'

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**Title** Collection of annotation related methods for mass spectrometry data

**Author** Carsten Kuhl, Ralf Tautenhahn, Steffen Neumann {ckuhl|sneumann}@ipb-halle.de, rtautenh@scripps.edu

**Maintainer** Steffen Neumann <sneumann@ipb-halle.de>

**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, 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

**NeedsCompilation** yes

## R topics documented:

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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,
  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](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](xsAnnotate-class).

## Author(s)

Carsten Kuhl <ckuhl@ipb-halle.de>

## Examples

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

---

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

---

## Description

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

## Usage

```
annotateDiffreport(object, sample=NA, nSlaves=1, sigma=6, perfwhm=0.6,
  cor_eic_th=0.75, cor_exp_th = 0.75, graphMethod="hcs", pval=0.05, 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 |
| psg_list | Calculation will only be done for the selected groups |
| rules | findAdducts: User defined ruleset |
| polarity | findAdducts: Which polarity mode was used for measuring of the ms sample |
| multiplier | findAdducts: If no ruleset is provided, calculate ruleset with max. number n of [nM+x] clusterions |
| max_peaks | How much peaks will be calculated in every thread using the parallel mode |
| intval | General used intensity value (into, maxo, intb) |
| pval_th | pval threshold. Creates a new psg_list. A pseudospectra is selected if it contains peaks, with pval < pval_th |
| fc_th | Same as pval. Select those groups with contains peaks with fold-change > fc_th. Pval_th and fc_th can be combined |
| sortpval | Sort diffreport after pvalues |
| ... | Diffreport parameters see [diffreport](#) |

## Details

Batch script wrapper for combining the annotation and the diffreport for a (grouped) xcmsSet xs. Function list: 1: diffreport(), 2: groupFWHM(), 3: findIsotopes(), 4: groupCorr(), 5: findAdducts() For a speedup calculation users can create a quick run, with quick = TRUE to preselect pseudospectra of interest. The indices of those pseudospectra are set with psg_list in a second run. On the other hand, a automatic selection with pval_th and/or fc_th can be performed. Returns the normal xcms diffreport table, with the additional CAMERA slots

## Value

annotateDiffreport returns an diffreport, see [diffreport](#), within additional columns containing the annotation results.

## Author(s)

Carsten Kuhl <ckuhl@ipb-halle.de>

## Examples

```
 #Multiple sample
 library(CAMERA)
 library(faahKO)
 xs.grp     <- group(faahko)
 xs.fill    <- fillPeaks(xs.grp)

 #fast preselection
# diffreport  <- annotateDiffreport(xs.fill,quick=TRUE)
# index <- c(1,18,35,45,56) #Make only for those grps a adduct annotation
```

```
# diffreport2 <- annotateDiffreport(xs.fill,psg_list=index,metlin = TRUE)

 #automatic selection for groups with peaks p-val < 0.05 and fold-change > 3
# diffreport <- annotateDiffreport(xs.fill,pval_th=0.05,fc=3)
```

---

calcCaS-methods              *EIC correlation grouping of LC/ESI-MS data*

---

## 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

```
library(CAMERA)
#Multiple sample
library(faahKO)
xs.grp        <- group(faahko)
#create xsAnnotate object
xsa           <- xsAnnotate(xs.grp)
#generate pseudospectra
xsa.group     <- groupFWHM(xsa)
#calculate correlation
correlationMatrix <- calcCaS(xsa.group)
```

---

calcCiS-methods *Calculate peak distance matrix after EIC correlation*

---

## Description

Processing an xsAnnotate object and correlates peak EIC curves from one pseudospectrum, using a precalculated EIC matrix ([getAllPeakEICs](#)). It return a weighted edge list as distance matrix between peaks according to the correlation analysis. The edge value is the pearson correlation coefficent. The list can be used as input for [calcPC](#).

## Usage

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

## Value

A matrix with 4 columns:

| | |
|---|---|
| x | peak index |
| y | peak index |
| cor | correlation value |
| ps | pseudospectrum index, which contains x and y |

## Author(s)

Carsten Kuhl <ckuhl@ipb-halle.de>

## See Also

[calcCaS](#) [groupCorr](#) [getAllPeakEICs](#) [xsAnnotate-class](#)

---

calcIsotopes-methods   *Calculate isotope distance matrix from xsAnnotate object*

---

## Description

Processing an xsAnnotate object with annotated isotopes ([findIsotopes](#)). It return a weighted edge list as distance matrix between peaks according to the isotope annotation. The edge value for recognized isotopes is 1 for all cases. The list can be used as input for [calcPC](#).

## Arguments

| | |
|---|---|
| object | xsAnnotate object |

## Value

A matrix with 4 columns:

| | |
|---|---|
| x | peak index |
| y | peak index |
| cor | edge value, always 1 |
| ps | pseudospectrum index, which contains x and y |

## Methods

**object = "xsAnnotate"**      calcIsotopes(object)

## Author(s)

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

## See Also

[calcPC](#) [xsAnnotate-class](#)

---

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](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](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](calcPC.hcs).

Further arguments given by `...` are passed through to the function implementing the `method`, which are most likely ajc. The parameter ajc is the peak distance matrix.

getOption("BioC")$CAMERA$findPeaks.methods returns a character vector of *nicknames* for the algorithms available.

The function returns a xsAnnotate object with grouping information, as list of peak indices. They are stored as object@pspectra.

### See Also

[calcPC.lpc](calcPC.lpc) [calcPC.hcs](calcPC.hcs) [xsAnnotate-class](xsAnnotate-class)

---

calcPC.hcs                           *Peakclustering into pseudospectra with the highly connected sub-graphs approach*

---

### Description

Cluster peaks from an xsAnnotate object into pseudospectra

### Arguments

object          xsAnnotate object

ajc             Weighted symbolic edge list as four column matrix ("x","y","cor","ps"). Columns
                x,y are peak indices, cor the edge value and ps the pseudospectrum index, where
                both peaks occur.

psg_list        additional vector ps pseudospectra indices, which are used in the clustering. If
                set to NULL all pseudospectra will be processed.

### Details

In some cases, is the peak grouping after retentiontime with [groupFWHM](#) not enough to separate
co-elution compounds. Therefore [groupCorr](#) use additional correlation analysis to achieve a 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.hcs(object, ajc=NULL, psg_list=NULL)

### Author(s)

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

### See Also

[calcPC](#) [groupCorr](#) [highlyConnSG](#) [xsAnnotate-class](#)

---

calcPC.lpc                           *Peakclustering into pseudospectra with the label-propagation-community algorithm*

---

### Description

Cluster peaks from an xsAnnotate object into pseudospectra

## Arguments

| | |
|---|---|
| object | xsAnnotate object |
| ajc | Weighted symbolic edge list as four column matrix ("x","y","cor","ps"). Columns x,y are peak indices, cor the edge value and ps the pseudospectrum index, where both peaks occur. |
| psg_list | additional vector ps pseudospectra indices, which are used in the clustering. If set to NULL all pseudospectra will be processed. |

## Details

In some cases, is the peak grouping after retentiontime with [groupFWHM](#) not enough to separate co-elution compounds. Therefore [groupCorr](#) use additional correlation analysis to achieve a separation. calcPC is part of this approach, which takes the calculated weighted edge list and performs the graph clustering. It returns an xsAnnotate object with further separated pseudospectra.

## Methods

**object = "xsAnnotate"**        calcPC.lpc(object, ajc=NULL, psg_list=NULL)

## Author(s)

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

## See Also

[calcPC](#) [groupCorr](#) [xsAnnotate-class](#) [label.propagation.community](#)

---

| cleanParallel | *Cleans up with spawned slave processes after use* |
|---|---|

---

## Description

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

## Usage

```
cleanParallel(object)
```

## Arguments

| | |
|---|---|
| object | xsAnnotate object |

## Details

The function needs a xsAnnotate object after groupCorr or groupFWHM. The resulting object is a artificial xcmsSet, where the peaks with the specific neutral loss are stored in xcmsSet@peaks.

**Author(s)**

Carsten Kuhl <ckuhl@ipb-halle.de>

**Examples**

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

## End(Not run)
```

---

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

---

**Description**

This function check 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**

```
    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 neagtive 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.

## Author(s)

Carsten Kuhl <ckuhl@ipb-halle.de>

## Examples

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

## End(Not run)
```

---

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 |

## Details

Adducts (and fragments) are annotated for a xsAnnotate object. For every pseudospectra group, generated bei groupFWHM and groupCorr, all possible Adducts are calculated and mapped to the peaks. If at least two adducts match, a possible molecule-mass for the group can be calculated. After the annotation every masshypothese is checked against the charge of the calculated isotopes. It is recommend to call findIsotopes() before the annotation step.

## Author(s)

Carsten Kuhl <ckuhl@ipb-halle.de>

## Examples

```
library(CAMERA)
file <- system.file('mzdata/MM14.mzdata', package = "CAMERA")
xs   <- xcmsSet(file, method="centWave", ppm=30, peakwidth=c(5,10))
an   <- xsAnnotate(xs)
an   <- groupFWHM(an)
an <- findIsotopes(an)  # optional but recommended.
#an <- groupCorr(an) # optional but very recommended step
an <- findAdducts(an,polarity="positive")
peaklist <- getPeaklist(an) # get the annotated peak list
```

---

findIsotopes                    *Deconvolute/Annotate LC/ESI-MS data*

---

## Description

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

## Usage

```
findIsotopes(object, maxcharge=3, maxiso=4, ppm=5, mzabs=0.01, intval=c("maxo","into","intb"), minf
```

## Arguments

| | |
|---|---|
| object | the xsAnnotate object |
| maxcharge | max. number of the isotope charge |
| maxiso | max. number of the isotope peaks |
| ppm | ppm error for the search |
| mzabs | allowed variance for the search |
| intval | choose intensity values for C12/C13 check. Allowed values are into, maxo, intb |
| minfrac | in case of multiple samples, percentaged value of samples, which have to contain the correct C12/C13 ratio and are not NA |
| isotopeMatrix | four column m/z-diff and ratio Matrix, for matching isotopic peaks. |
| filter | Should C12/C13 filter be applied |

## Details

Isotope peaks are annotated for a xsAnnotate object according to given rules (maxcharge, maxiso). The algorithm benefits from a earlier grouping of the data, with groupFWHM. Generates a list of all possible isotopes, which is stored in object@isotopes. Those isotope information will be used in the groupCorr funtion. The itensity of the C13 isotope peak is checked against the C12 of proper ratio. In the case of mulitiple 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)
```

---

findKendrickMasses    *Find specfic 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 |

## 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)
```

---

getAllPeakEICs          *Generate EIC information from raw data*

---

### Description

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

### Usage

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

### 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 acessable. 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](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;
```

getIsotopeCluster          *Retrieve the annotatad 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)

#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)
```

---

getPeaklist                  *Generate the annotatad 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

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

---

getpspectra                 *Retrieve a peaklist of one or more pseudospectra*

---

## Description

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

## Usage

```
getpspectra(object, grp)
```

## Arguments

| | |
|---|---|
| object | xsAnnotate object |
| grp | index of pseudo-spectra-group |

## Details

xsAnnotate groups LC/MS Peaklist after 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, calcCiS = TRUE, calcCaS = FALSE, psg_list=NULL, xraw=NULL,
cor_exp_th=0.75, ...)
```

## Arguments

| | |
|---|---|
| object | The xsAnnotate object |
| cor_eic_th | Correlation threshold for EIC correlation |
| pval | p-value threshold for testing correlation of significance |
| graphMethod | Clustering method for resulting correlation graph. See calcPC for more details. |
| calcIso | Include isotope detection informationen for graph clustering |
| calcCiS | Calculate correlation inside samples |
| calcCaS | Calculate correlation accross samples |
| psg_list | Vector of pseudospectra indices. The correlation analysis will be only done for those groups |
| xraw | Optional xcmsRaw object, which should be used for raw data extraction |
| cor_exp_th | Threshold for intensity correlations across samples |
| ... | 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 informationen 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**

```
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.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

```
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 there 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 eluate at the same time-point as a selected peak, will be part of the group. Same time-point is defined about the Rt_med +/- FWHM * perfwhm. For a single sample xcmsSet the selection of peaks starts at the most abundant and goes down to the smaller ones. With a multiple sample set the automatic selection uses the most abundant peak as an representative for every feature group, according to the xcms grouping. With the xsAnnotate sample parameter a sample selection can be defined to use only specific samples. See [xsAnnotate-class](xsAnnotate-class) for further information. The FWHM (full width at half maximum) of a peak is estimated as FWHM = SD * 2.35. For the calculation of the SD, the peak is assumed as normal distributed.

### Author(s)

Carsten Kuhl <ckuhl@ipb-halle.de>

### Examples

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

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

#With specific selected sample
xs.anno  <- xsAnnotate(xs, sample=1)
xs.group <- groupFWHM(xs.anno)

#With automatic selection
xs.anno.auto  <- xsAnnotate(xs)
xs.group.auto <- groupFWHM(xs.anno.auto)
```

---

mm14 *Extract of marker mixture 14 LC/MS data*

---

### Description

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

### Usage

```
data(mm14)
```

### Format

The format is:

```
Formal class 'xcmsSet' [package "xcms"] with 8 slots
    @ peaks    : num [1:83, 1:11] 117 117 118 119 136
  .. ..- attr(*, "dimnames")=List of 2
  .. .. ..$ : NULL
  .. .. ..$ : chr [1:11] "mz" "mzmin" "mzmax" "rt"
  ..@ groups   : logi[0 , 0 ]
  ..@ groupidx : list()
  ..@ phenoData:'data.frame': 1 obs. of  1 variable:
  .. ..$ class: Factor w/ 1 level "mzdata": 1
  ..@ rt       :List of 2
  .. ..$ raw      :List of 1
```

```
.. .. ..$ : num [1:112] 270 271 271 271 272 ...
.. ..$ corrected:List of 1
.. .. ..$ : num [1:112] 270 271 271 271 272 ...
..@ filepaths: chr "mzdata/MM14.mzdata"
..@ profinfo :List of 2
.. ..$ method: chr "bin"
.. ..$ step  : num 0.1
..@ polarity : chr(0)
```

### Details

The corresponding raw mzData files are located in the mzData subdirectory of this package.

### Author(s)

Carsten Kuhl <ckuhl@ipb-halle.de>

### Source

http://doi:10.1186/1471-2105-9-504

### References

Data originally reported in "Highly sensitive feature detection for high resolution LC/MS" BMC Bioinformatics; 2008; 9:504.

---

plotEICs-methods          *Plot extracted ion chromatograms from (multiple) Pseudospectra*

---

### Description

Batch plot a list of extracted ion chromatograms to the current graphics device.

### Arguments

| | |
|---|---|
| object | the xsAnnotate object |
| xraw | xcmsRaw object underlying the the xsAnnotate |
| maxlabel | How many m/z labels to print |
| sleep | seconds to pause between plotting EICs |
| ... | other graphical parameters |

### Value

None.

## Methods

**object = "xsAnnotate"**     plotEICs(object,   xraw,   pspec=1:length(object@pspectra),   maxlabel=0, s

## Author(s)

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

## See Also

[xsAnnotate-class](), [png](), [pdf](), [postscript](),

---

plotPsSpectrum-methods

*Plot a Pseudospectrum*

---

### Description

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

### Usage

    plotPsSpectrum(object, pspec=1:length(object@pspectra), log=FALSE, value="into", maxlabel=0, title=

### 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](),

---

psDist-methods               *Distance methods for xsAnnotate*

---

### Description

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

### Arguments

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

### Details

Different algorithms can be used by specifying them with the method argument. For example to use the "meanMZmatch" approach one would use: specDist(object1, object2, pspectrum1, pspectrum2, method="mean 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")$xcms$specDis 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, expecially from tandem-MS, but also in-source fragments might give additional hints on top of the accurate mass of the precursor alone.

**Usage**

```
pspec2metfrag(object, pspecidx=NULL, filedir=NULL)
pspec2metfusion(object, pspecidx=NULL, filedir=NULL)
```

**Arguments**

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

**Details**

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

**Value**

Returns a list

**Author(s)**

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 step
an          <- findAdducts(an, polarity="positive")

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

---

ruleSet                  *Class* ruleSet

---

### Description

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

### Slots

ionlistfile: File of known charged ions, an example is found in CAMERA/lists/ions.csv .

neutrallossfile: File of known neutral losses, an example is found in CAMERA/lists/neutralloss.csv.

neutraladditionfile: File of known adducts, an example is found in CAMERA/lists/lists/neutraladdition.csv .

ionlist: Known charged ions.

neutralloss: Known neutral losses.

neutraladdition: Known adducts.

maxcharge: .

mol : .

nion : .

nnloss : .

nnadd : .

nh : .

polarity : Polarity of the ruleSet.

rules: data.frame of resulting mass differences, this is the dynamic ruleSet.

lib.loc  Path to local R library

### Extends

Class "Versioned", directly.

### Methods

Methods implemented for ruleSet

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

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

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

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

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

## Author(s)

Steffen Neumann and Carsten Kuhl

## Examples

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

---

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 needs the raw data a selection algorithm must be choosen in the case of a multiple sample. CAMERA includes two different strategies: A defined selection of samples (sample = indices of samples) or the default automatic solution (sample = NA). The automatic solution chooses the best sample for a specifc 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)
```

---

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 algorihms 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 pro-
vided [xcmsSet](#). Objects can also be created by calls of the form new("xsAnnotate", ...).

#### Slots

annoGrp: Assignment of mass hypotheses to correlation groups

annoID: The assignemnt of peaks to the mass difference rule used

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 annotion

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

# Index