Package 'xcms'

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Title LC/MS and GC/MS Data Analysis

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Description Framework for processing and visualization of chromatographically
separated and single-spectra mass spectral data. Imports from AIA/ANDI NetCDF,
mzXML, mzData and mzML files. Preprocesses data for high-throughput, untargeted
analyte profiling.

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URL http://metlin.scripps.edu/download/ and
https://github.com/sneumann/xcms

VignetteBuilder knitr

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

biocViews MassSpectrometry, Metabolomics

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Collate 'AllGenerics.R' 'DataClasses.R' 'Deprecated.R' 'MPI.R' 'c.R'
'cwTools.R' 'databases.R' 'functions-MsFeatureData.R'
'do_adjustRtime-functions.R' 'functions-binning.R'
'do_findChromPeaks-functions.R' 'functions-Params.R'
'do_groupChromPeaks-functions.R' 'fastMatch.R'

'functions-utils.R' 'functions-IO.R' 'functions-OnDiskMSnExp.R'
'functions-ProcessHistory.R' 'functions-XCMSnExp.R'
'functions-normalization.R' 'functions-xcmsEIC.R'
'functions-xcmsFragments.R' 'functions-xcmsRaw.R'
'functions-xcmsSet.R' 'init.R' 'matchpeaks.R' 'methods-IO.R'
'methods-MsFeatureData.R' 'methods-OnDiskMSnExp.R'
'methods-Params.R' 'methods-ProcessHistory.R'
'methods-XCMSnExp.R' 'methods-netCdfSource.R'
'methods-rampSource.R' 'methods-xcmsEIC.R'
'methods-xcmsFileSource.R' 'methods-xcmsFragments.R'
'methods-xcmsPeaks.R' 'methods-xcmsRaw.R' 'methods-xcmsSet.R'
'models.R' 'msn2xcmsRaw.R' 'mzClust.R' 'netCDF.R' 'plotQC.R'
'ramp.R' 'specDist.R' 'write.mzquantML.R' 'writemzdata.R'
'writemztab.R' 'xcmsSource.R' 'zzz.R'

NeedsCompilation yes

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absent-methods *Determine which peaks are absent / present in a sample class*

Description

Determine which peaks are absent / present in a sample class

Arguments

object	xcmsSet-class object
class	Name of a sample class from sampclass
minfrac	minimum fraction of samples necessary in the class to be absent/present

Details

Determine which peaks are absent / present in a sample class The functions treat peaks that are only present because of fillPeaks correctly, i.e. does not count them as present.

Value

An logical vector with the same length as nrow(groups(object)).

Methods

object = "xcmsSet" absent(object, ...) present(object, ...)

See Also

group diffreport

adjustRtime *Alignment: Retention time correction methods.*

Description

The adjustRtime method(s) perform retention time correction (alignment) between chromatograms of different samples. These methods are part of the modernized xcms user interface.

The implemented retention time adjustment methods are:

peakGroups retention time correction based on aligment of features (peak groups) present in most/all samples. See adjustRtime-peakGroups for more details.

obiwarp alignment based on the complete mz-rt data. This method does not require any identified peaks or defined features. See adjustRtime-obiwarp for more details.

Author(s)

Johannes Rainer

See Also

retcor for the *old* retention time correction methods. plotAdjustedRtime for visualization of alignment results.

Other retention time correction methods: adjustRtime-obiwarp, adjustRtime-peakGroups

---

adjustRtime-obiwarp *Align retention times across samples using Obiwarp*

Description

This method performs retention time adjustment using the Obiwarp method [Prince 2006]. It is based on the code at http://obi-warp.sourceforge.net but supports alignment of multiple samples by aligning each against a *center* sample. The alignment is performed directly on the profile-matrix and can hence be performed independently of the peak detection or peak grouping.

The ObiwarpParam class allows to specify all settings for the retention time adjustment based on the *obiwarp* method. Class Instances should be created using the ObiwarpParam constructor.

binSize,binSize<-: getter and setter for the binSize slot of the object.

centerSample,centerSample<-: getter and setter for the centerSample slot of the object.

response,response<-: getter and setter for the response slot of the object.

distFun,distFun<-: getter and setter for the distFun slot of the object.

gapInit,gapInit<-: getter and setter for the gapInit slot of the object.

gapExtend,gapExtend<-: getter and setter for the gapExtend slot of the object.

factorDiag,factorDiag<-: getter and setter for the factorDiag slot of the object.

factorGap,factorGap<-: getter and setter for the factorGap slot of the object.

localAlignment,localAlignment<-: getter and setter for the localAlignment slot of the object.

initPenalty,initPenalty<-: getter and setter for the initPenalty slot of the object.

adjustRtime,XCMSnExp,ObiwarpParam: performs retention time correction/alignment based on the total mz-rt data using the *obiwarp* method.

Usage

```
ObiwarpParam(binSize = 1, centerSample = integer(), response = 1L,
  distFun = "cor_opt", gapInit = numeric(), gapExtend = numeric(),
  factorDiag = 2, factorGap = 1, localAlignment = FALSE,
  initPenalty = 0)

## S4 method for signature 'OnDiskMSnExp,ObiwarpParam'
adjustRtime(object, param, msLevel = 1L)

## S4 method for signature 'ObiwarpParam'
show(object)

## S4 method for signature 'ObiwarpParam'
binSize(object)
```

```
## S4 replacement method for signature 'ObiwarpParam'
binSize(object) <- value

## S4 method for signature 'ObiwarpParam'
centerSample(object)

## S4 replacement method for signature 'ObiwarpParam'
centerSample(object) <- value

## S4 method for signature 'ObiwarpParam'
response(object)

## S4 replacement method for signature 'ObiwarpParam'
response(object) <- value

## S4 method for signature 'ObiwarpParam'
distFun(object)

## S4 replacement method for signature 'ObiwarpParam'
distFun(object) <- value

## S4 method for signature 'ObiwarpParam'
gapInit(object)

## S4 replacement method for signature 'ObiwarpParam'
gapInit(object) <- value

## S4 method for signature 'ObiwarpParam'
gapExtend(object)

## S4 replacement method for signature 'ObiwarpParam'
gapExtend(object) <- value

## S4 method for signature 'ObiwarpParam'
factorDiag(object)

## S4 replacement method for signature 'ObiwarpParam'
factorDiag(object) <- value

## S4 method for signature 'ObiwarpParam'
factorGap(object)

## S4 replacement method for signature 'ObiwarpParam'
factorGap(object) <- value

## S4 method for signature 'ObiwarpParam'
localAlignment(object)

## S4 replacement method for signature 'ObiwarpParam'
localAlignment(object) <- value

## S4 method for signature 'ObiwarpParam'
```

```
initPenalty(object)

## S4 replacement method for signature 'ObiwarpParam'
initPenalty(object) <- value

## S4 method for signature 'XCMSnExp,ObiwarpParam'
adjustRtime(object, param, msLevel = 1L)
```

Arguments

binSize	numeric(1) defining the bin size (in mz dimension) to be used for the *profile matrix* generation. See step parameter in profile-matrix documentation for more details.
centerSample	integer(1) defining the index of the center sample in the experiment. It defaults to floor(median(1:length(fileNames(object)))).
response	numeric(1) defining the *responsiveness* of warping with response = 0 giving linear warping on start and end points and response = 100 warping using all bijective anchors.
distFun	character defining the distance function to be used. Allowed values are "cor" (Pearson's correlation), "cor_opt" (calculate only 10% diagonal band of distance matrix; better runtime), "cov" (covariance), "prd" (product) and "euc" (Euclidian distance). The default value is distFun = "cor_opt".
gapInit	numeric(1) defining the penalty for gap opening. The default value for gapInit depends on the value of distFun: for distFun = "cor" and distFun = "cor_opt" it is 0.3, for distFun = "cov" and distFun = "prd" 0.0 and for distFun = "euc" 0.9.
gapExtend	numeric(1) defining the penalty for gap enlargement. The default value for gapExtend depends on the value of distFun, for distFun = "cor" and distFun = "cor_opt" it is 2.4, for distFun = "cov" 11.7, for distFun = "euc" 1.8 and for distFun = "prd" 7.8.
factorDiag	numeric(1) defining the local weight applied to diagonal moves in the alignment.
factorGap	numeric(1) defining the local weight for gap moves in the alignment.
localAlignment	logical(1) whether a local alignment should be performed instead of the default global alignment.
initPenalty	numeric(1) defining the penalty for initiating an alignment (for local alignment only).
object	For adjustRtime: an XCMSnExp object. For all other methods: a ObiwarpParam object.
param	A ObiwarpParam object containing all settings for the alignment method.
msLevel	integer defining the MS level on which the retention time should be performed.
value	The value for the slot.

Value

The ObiwarpParam function returns a ObiwarpParam class instance with all of the settings specified for obiwarp retention time adjustment and alignment.

For adjustRtime,XCMSnExp,ObiwarpParam: a XCMSnExp object with the results of the retention time adjustment step. These can be accessed with the adjustedRtime method. Retention time

correction does also adjust the retention time of the identified chromatographic peaks (accessed *via* chromPeaks. Note that retention time correction drops all previous peak grouping results from the result object.

For adjustRtime,OnDiskMSnExp,ObiwarpParam: a numeric with the adjusted retention times per spectra (in the same order than rtime).

Slots

.__classVersion__,binSize,centerSample,response,distFun,gapInit,gapExtend,factorDiag,factorGap,l
: See corresponding parameter above. .__classVersion__ stores the version from the class. Slots values should exclusively be accessed *via* the corresponding getter and setter methods listed above.

Note

These methods and classes are part of the updated and modernized xcms user interface which will eventually replace the retcor methods. All of the settings to the alignment algorithm can be passed with a ObiwarpParam object.

Alignment using obiwarp is performed on the retention time of spectra of on MS level. Retention times for spectra of other MS levels are subsequently adjusted based on the adjustment function defined on the retention times of the spectra of MS level msLevel.

Calling adjustRtime on an XCMSnExp object will cause all peak grouping (correspondence) results and any previous retention time adjustment results to be dropped.

Author(s)

Colin Smith, Johannes Rainer

References

John T. Prince and Edward M. Marcotte. "Chromatographic Alignment of ESI-LC-MS Proteomics Data Sets by Ordered Bijective Interpolated Warping" *Anal. Chem.* 2006, 78(17):6140-6152.

John T. Prince and Edward M. Marcotte. "Chromatographic Alignment of ESI-LC-MS Proteomic Data Sets by Ordered Bijective Interpolated Warping" *Anal. Chem.* 2006, 78 (17), 6140-6152.

See Also

retcor.obiwarp for the old user interface. plotAdjustedRtime for visualization of alignment results.

XCMSnExp for the object containing the results of the alignment.

Other retention time correction methods: adjustRtime-peakGroups, adjustRtime

Examples

```
library(faahKO)
library(MSnbase)
fls <- dir(system.file("cdf/KO", package = "faahKO"), recursive = TRUE,
           full.names = TRUE)

## Reading 2 of the KO samples
raw_data <- readMSData(fls[1:2], mode = "onDisk")

## Perform retention time correction on the OnDiskMSnExp:
```

```
res <- adjustRtime(raw_data, param = ObiwarpParam())

## As a result we get a numeric vector with the adjusted retention times for
## all spectra.
head(res)

## We can split this by file to get the adjusted retention times for each
## file
resL <- split(res, fromFile(raw_data))

##############################
## Perform retention time correction on an XCMSnExp:
##
## Perform first the chromatographic peak detection using the matchedFilter
## method.
mfp <- MatchedFilterParam(snthresh = 20, binSize = 1)
res <- findChromPeaks(raw_data, param = mfp)

## Performing the retention time adjustment using obiwarp.
res_2 <- adjustRtime(res, param = ObiwarpParam())

head(rtime(res_2))
head(rtime(raw_data))

## Also the retention times of the detected peaks were adjusted.
tail(chromPeaks(res))
tail(chromPeaks(res_2))
```

`adjustRtime-peakGroups` *Retention time correction based on alignment of house keeping peak groups*

Description

This method performs retention time adjustment based on the alignment of chromatographic peak groups present in all/most samples (hence corresponding to house keeping compounds). First the retention time deviation of these peak groups is described by fitting either a polynomial (`smooth = "loess"`) or a linear (`smooth = "linear"`) model to the data points. These models are subsequently used to adjust the retention time of each spectrum in each sample.

The `PeakGroupsParam` class allows to specify all settings for the retention time adjustment based on *house keeping* peak groups present in most samples. Instances should be created with the `PeakGroupsParam` constructor.

`adjustRtimePeakGroups` returns the features (peak groups) which would, depending on the provided `PeakGroupsParam`, be selected for alignment/retention time correction.

`minFraction`,`minFraction<-`: getter and setter for the `minFraction` slot of the object.

`extraPeaks`,`extraPeaks<-`: getter and setter for the `extraPeaks` slot of the object.

`smooth`,`smooth<-`: getter and setter for the `smooth` slot of the object.

`span`,`span<-`: getter and setter for the `span` slot of the object.

`family`,`family<-`: getter and setter for the `family` slot of the object.

peakGroupsMatrix,peakGroupsMatrix<-: getter and setter for the peakGroupsMatrix slot of the object.

adjustRtime,XCMSnExp,PeakGroupsParam: performs retention time correction based on the alignment of peak groups (features) found in all/most samples. The correction function identified on these peak groups is applied to the retention time of all spectra in the object, i.e. retention times of all spectra, also MS level > 1 are adjusted.

Usage

```
PeakGroupsParam(minFraction = 0.9, extraPeaks = 1, smooth = "loess",
  span = 0.2, family = "gaussian", peakGroupsMatrix = matrix(nrow = 0,
  ncol = 0))

adjustRtimePeakGroups(object, param = PeakGroupsParam())

## S4 method for signature 'PeakGroupsParam'
show(object)

## S4 method for signature 'PeakGroupsParam'
minFraction(object)

## S4 replacement method for signature 'PeakGroupsParam'
minFraction(object) <- value

## S4 method for signature 'PeakGroupsParam'
extraPeaks(object)

## S4 replacement method for signature 'PeakGroupsParam'
extraPeaks(object) <- value

## S4 method for signature 'PeakGroupsParam'
smooth(x)

## S4 replacement method for signature 'PeakGroupsParam'
smooth(object) <- value

## S4 method for signature 'PeakGroupsParam'
span(object)

## S4 replacement method for signature 'PeakGroupsParam'
span(object) <- value

## S4 method for signature 'PeakGroupsParam'
family(object)

## S4 replacement method for signature 'PeakGroupsParam'
family(object) <- value

## S4 method for signature 'PeakGroupsParam'
peakGroupsMatrix(object)

## S4 replacement method for signature 'PeakGroupsParam'
```

```
peakGroupsMatrix(object) <- value

## S4 method for signature 'XCMSnExp,PeakGroupsParam'
adjustRtime(object, param)
```

Arguments

minFraction	numeric(1) between 0 and 1 defining the minimum required fraction of samples in which peaks for the peak group were identified. Peak groups passing this criteria will aligned across samples and retention times of individual spectra will be adjusted based on this alignment. For minFraction = 1 the peak group has to contain peaks in all samples of the experiment.
extraPeaks	numeric(1) defining the maximal number of additional peaks for all samples to be assigned to a peak group (i.e. feature) for retention time correction. For a data set with 6 samples, extraPeaks = 1 uses all peak groups with a total peak count <= 6 + 1. The total peak count is the total number of peaks being assigned to a peak group and considers also multiple peaks within a sample being assigned to the group.
smooth	character defining the function to be used, to interpolate corrected retention times for all peak groups. Either "loess" or "linear".
span	numeric(1) defining the degree of smoothing (if smooth = "loess"). This parameter is passed to the internal call to loess.
family	character defining the method to be used for loess smoothing. Allowed values are "gaussian" and "symmetric".See loess for more information.
peakGroupsMatrix	optional matrix of (raw) retention times for the peak groups on which the alignment should be performed. Each column represents a sample, each row a feature/peak group. Such a matrix is for example returned by the adjustRtimePeakGroups method.
object	For adjustRtime: an XCMSnExp object containing the results from a previous chromatographic peak detection (see findChromPeaks) and alignment analysis (see groupChromPeaks). For all other methods: a PeakGroupsParam object.
param	A PeakGroupsParam object containing all settings for the retention time correction method..
value	The value for the slot.
x	a PeakGroupsParam object.

Value

The PeakGroupsParam function returns a PeakGroupsParam class instance with all of the settings specified for retention time adjustment based on *house keeping* features/peak groups.

For adjustRtimePeakGroups: a matrix, rows being features, columns samples, of retention times. The features are ordered by the median retention time across columns.

For adjustRtime: a XCMSnExp object with the results of the retention time adjustment step. These can be accessed with the adjustedRtime method. Retention time correction does also adjust the retention time of the identified chromatographic peaks (accessed *via* chromPeaks. Note that retention time correction drops all previous alignment results from the result object.

Slots

`.__classVersion__,minFraction,extraPeaks,smooth,span,family,peakGroupsMatrix` See corresponding parameter above. `.__classVersion__` stores the version from the class. Slots values should exclusively be accessed *via* the corresponding getter and setter methods listed above.

Note

These methods and classes are part of the updated and modernized `xcms` user interface which will eventually replace the `group` methods. All of the settings to the alignment algorithm can be passed with a `PeakGroupsParam` object.

The matrix with the (raw) retention times of the peak groups used in the alignment is added to the `peakGroupsMatrix` slot of the `PeakGroupsParam` object that is stored into the corresponding *process history step* (see `processHistory` for how to access the process history).

`adjustRtimePeakGroups` is supposed to be called *before* the sample alignment, but after a correspondence (peak grouping).

This method requires that a correspondence analysis has been performed on the data, i.e. that grouped chromatographic peaks/features are present (see `groupChromPeaks` for details).

Calling `adjustRtime` on an `XCMSnExp` object will cause all peak grouping (correspondence) results and any previous retention time adjustments to be dropped. In some instances, the `adjustRtime,XCMSnExp,PeakGroups` re-adjusts adjusted retention times to ensure them being in the same order than the raw (original) retention times.

Author(s)

Colin Smith, Johannes Rainer

References

Colin A. Smith, Elizabeth J. Want, Grace O'Maille, Ruben Abagyan and Gary Siuzdak. "XCMS: Processing Mass Spectrometry Data for Metabolite Profiling Using Nonlinear Peak Alignment, Matching, and Identification" *Anal. Chem.* 2006, 78:779-787.

See Also

The `do_adjustRtime_peakGroups` core API function and `retcor.peakgroups` for the old user interface. `plotAdjustedRtime` for visualization of alignment results.

`XCMSnExp` for the object containing the results of the alignment.

Other retention time correction methods: `adjustRtime-obiwarp`, `adjustRtime`

Examples

```
##############################
## Chromatographic peak detection and grouping.
##
## Below we perform first a peak detection (using the matchedFilter
## method) on some of the test files from the faahKO package followed by
## a peak grouping.
library(faahKO)
library(xcms)
fls <- dir(system.file("cdf/KO", package = "faahKO"), recursive = TRUE,
           full.names = TRUE)
```

```
## Reading 2 of the KO samples
raw_data <- readMSData(fls[1:2], mode = "onDisk")

## Perform the peak detection using the matchedFilter method.
mfp <- MatchedFilterParam(snthresh = 20, binSize = 1)
res <- findChromPeaks(raw_data, param = mfp)

head(chromPeaks(res))
## The number of peaks identified per sample:
table(chromPeaks(res)[, "sample"])

## Performing the peak grouping using the "peak density" method.
p <- PeakDensityParam(sampleGroups = c(1, 1))
res <- groupChromPeaks(res, param = p)

## Perform the retention time adjustment using peak groups found in both
## files.
fgp <- PeakGroupsParam(minFraction = 1)

## Before running the alignment we can evaluate which features (peak groups)
## would be used based on the specified parameters.
pkGrps <- adjustRtimePeakGroups(res, param = fgp)

## We can also plot these to evaluate if the peak groups span a large portion
## of the retention time range.
plot(x = pkGrps[, 1], y = rep(1, nrow(pkGrps)), xlim = range(rtime(res)),
    ylim = c(1, 2), xlab = "rt", ylab = "", yaxt = "n")
points(x = pkGrps[, 2], y = rep(2, nrow(pkGrps)))
segments(x0 = pkGrps[, 1], x1 = pkGrps[, 2],
    y0 = rep(1, nrow(pkGrps)), y1 = rep(2, nrow(pkGrps)))
grid()
axis(side = 2, at = c(1, 2), labels = colnames(pkGrps))

## Next we perform the alignment.
res <- adjustRtime(res, param = fgp)

## Any grouping information was dropped
hasFeatures(res)

## Plot the raw against the adjusted retention times.
plot(rtime(raw_data), rtime(res), pch = 16, cex = 0.25, col = fromFile(res))

## Adjusterd retention times can be accessed using
## rtime(object, adjusted = TRUE) and adjustedRtime
all.equal(rtime(res), adjustedRtime(res))

## To get the raw, unadjusted retention times:
all.equal(rtime(res, adjusted = FALSE), rtime(raw_data))

## To extract the retention times grouped by sample/file:
rts <- rtime(res, bySample = TRUE)
```

---

applyAdjustedRtime *Replace raw with adjusted retention times*

Description

Replaces the raw retention times with the adjusted retention time or returns the object unchanged if none are present.

Usage

```
applyAdjustedRtime(object)
```

Arguments

object	An XCMSnExp object.

Details

Adjusted retention times are stored *in parallel* to the adjusted retention times in the XCMSnExp. The applyAdjustedRtime replaces the raw retention times (stored in the *feature data* (fData data.frame)) with the adjusted retention times.

Value

A XCMSnExp with the raw retention times being replaced with the adjusted retention time.

Note

Replacing the raw retention times with adjusted retention times disables the possibility to restore raw retention times using the dropAdjustedRtime() method. This function does **not** remove the retention time processing step with the settings of the alignment from the processHistory() of the object to ensure that the processing history is preserved.

Author(s)

Johannes Rainer

See Also

adjustRtime() for the function to perform the alignment (retention time correction).

[adjustedRtime()] for the method to extract adjusted retention times from an [XCMSnExp] object.

[dropAdjustedRtime] for the method to delete alignment results and to restore the raw retention times.

Examples

```
## Load test data
files <- c(system.file('cdf/KO/ko15.CDF', package = "faahKO"),
    system.file('cdf/KO/ko16.CDF', package = "faahKO"),
    system.file('cdf/KO/ko18.CDF', package = "faahKO"))

od <- readMSData(files, mode = "onDisk")

## Apply obiwarp retention time adjustment. We have to convert the
## OnDiskMSnExp first to an XCMSnExp
xod <- as(od, "XCMSnExp")
```

```
xod <- adjustRtime(xod, param = ObiwarpParam())

hasAdjustedRtime(xod)

## Replace raw retention times with adjusted retention times.
xod <- applyAdjustedRtime(xod)

## No adjusted retention times present
hasAdjustedRtime(xod)

## Raw retention times have been replaced with adjusted retention times
plot(split(rtime(od), fromFile(od))[[1]] -
    split(rtime(xod), fromFile(xod))[[1]], type = "l")

## And the process history still contains the settings for the alignment
processHistory(xod)
```

AutoLockMass-methods *Automatic parameter for Lock mass fixing* AutoLockMass ~~

Description

AutoLockMass - This function decides where the lock mass scans are in the xcmsRaw object. This is done by using the scan time differences.

Arguments

object	An xcmsRaw-class object

Value

AutoLockMass A numeric vector of scan locations corresponding to lock Mass scans

Methods

object = "xcmsRaw" signature(object = "xcmsRaw")

Author(s)

Paul Benton, <hpaul.benton08@imperial.ac.uk>

Examples

```
## Not run: library(xcms)
library(faahKO) ## These files do not have this problem to correct for but just for an example
cdfpath <- system.file("cdf", package = "faahKO")
cdffiles <- list.files(cdfpath, recursive = TRUE, full.names = TRUE)
xr<-xcmsRaw(cdffiles[1])
xr
##Lets assume that the lockmass starts at 1 and is every 100 scans
lockMass<-xcms:::makeacqNum(xr, freq=100, start=1)
## these are equalvent
lockmass2<-AutoLockMass(xr)
all((lockmass == lockmass2) == TRUE)
```

```
ob<-stitch(xr, lockMass)

## End(Not run)
```

`bin,XCMSnExp-method` *XCMSnExp data manipulation methods inherited from MSnbase*

Description

The methods listed on this page are `XCMSnExp` methods inherited from its parent, the `OnDiskMSnExp` class from the `MSnbase` package, that alter the raw data or are related to data subsetting. Thus calling any of these methods causes all `xcms` pre-processing results to be removed from the `XCMSnExp` object to ensure its data integrity.

`bin`: allows to *bin* spectra. See `bin` documentation for more details and examples.

`clean`: removes unused `0` intensity data points. See `clean` documentation for details and examples.

`filterAcquisitionNum`: filters the `XCMSnExp` object keeping only spectra with the provided acquisition numbers. See `filterAcquisitionNum` for details and examples.

The `normalize` method performs basic normalization of spectra intensities. See `normalize` documentation for details and examples.

The `pickPeaks` method performs peak picking. See `pickPeaks` documentation for details and examples.

The `removePeaks` method removes mass peaks (intensities) lower than a threshold. Note that these peaks refer to *mass* peaks, which are different to the chromatographic peaks detected and analyzed in a metabolomics experiment! See `removePeaks` documentation for details and examples.

The `smooth` method smooths spectra. See `smooth` documentation for details and examples.

Usage

```
## S4 method for signature 'XCMSnExp'
bin(object, binSize = 1L, msLevel.)

## S4 method for signature 'XCMSnExp'
clean(object, all = FALSE, verbose = FALSE, msLevel.)

## S4 method for signature 'XCMSnExp'
filterAcquisitionNum(object, n, file)

## S4 method for signature 'XCMSnExp'
normalize(object, method = c("max", "sum"), ...)

## S4 method for signature 'XCMSnExp'
pickPeaks(object, halfWindowSize = 3L,
  method = c("MAD", "SuperSmoother"), SNR = 0L, ...)

## S4 method for signature 'XCMSnExp'
removePeaks(object, t = "min", verbose = FALSE,
  msLevel.)
```

```
## S4 method for signature 'XCMSnExp'
smooth(x, method = c("SavitzkyGolay", "MovingAverage"),
  halfWindowSize = 2L, verbose = FALSE, ...)
```

Arguments

object	XCMSnExp or OnDiskMSnExp object.
binSize	numeric(1) defining the size of a bin (in Dalton).
msLevel.	For bin, clean, filterMsLevel, removePeaks: numeric(1) defining the MS level(s) to which operations should be applied or to which the object should be subsetted.
all	For clean: logical(1), if TRUE all zeros are removed.
verbose	logical(1) whether progress information should be displayed.
n	For filterAcquisitionNum: integer defining the acquisition numbers of the spectra to which the data set should be sub-setted.
file	For filterAcquisitionNum: integer defining the file index within the object to subset the object by file.
method	For normalize: character(1) specifying the normalization method. See normalize for details. For pickPeaks: character(1) defining the method. See pickPeaks for options. For smooth: character(1) defining the method. See smooth for options and details.
...	Optional additional arguments.
halfWindowSize	For pickPeaks and smooth: integer(1) defining the window size for the peak picking. See pickPeaks and smooth for details and options.
SNR	For pickPeaks: numeric(1) defining the signal to noise ratio to be considered. See pickPeaks documentation for details.
t	For removePeaks: either a numeric(1) or "min" defining the threshold (method) to be used. See removePeaks for details.
x	XCMSnExp or OnDiskMSnExp object.

Value

For all methods: a XCMSnExp object.

Author(s)

Johannes Rainer

See Also

XCMSnExp-filter for methods to filter and subset XCMSnExp objects. XCMSnExp for base class documentation. OnDiskMSnExp for the documentation of the parent class.

binYonX *Aggregate values in y for bins defined on x*

Description

This functions takes two same-sized numeric vectors x and y, bins/cuts x into bins (either a pre-defined number of equal-sized bins or bins of a pre-defined size) and aggregates values in y corresponding to x values falling within each bin. By default (i.e. `method = "max"`) the maximal y value for the corresponding x values is identified. x is expected to be incrementally sorted and, if not, it will be internally sorted (in which case also y will be ordered according to the order of x).

Usage

```
binYonX(x, y, breaks, nBins, binSize, binFromX, binToX, fromIdx = 1L,
  toIdx = length(x), method = "max", baseValue, sortedX = !is.unsorted(x),
  shiftByHalfBinSize = FALSE, returnIndex = FALSE, returnX = TRUE)
```

Arguments

x	Numeric vector to be used for binning.
y	Numeric vector (same length than x) from which the maximum values for each bin should be defined. If not provided, x will be used.
breaks	Numeric vector defining the breaks for the bins, i.e. the lower and upper values for each bin. See examples below.
nBins	integer(1) defining the number of desired bins.
binSize	numeric(1) defining the desired bin size.
binFromX	Optional numeric(1) allowing to manually specify the range of x-values to be used for binning. This will affect only the calculation of the breaks for the bins (i.e. if nBins or binSize is provided). If not provided the minimal value in the sub-set fromIdx-toIdx in input vector x will be used.
binToX	Same as binFromX, but defining the maximum x-value to be used for binning.
fromIdx	Integer vector defining the start position of one or multiple sub-sets of input vector x that should be used for binning.
toIdx	Same as toIdx, but defining the maximum index (or indices) in x to be used for binning.
method	A character string specifying the method that should be used to aggregate values in y. Allowed are "max", "min", "sum" and "mean" to identify the maximal or minimal value or to sum all values within a bin or calculate their mean value.
baseValue	The base value for empty bins (i.e. bins into which either no values in x did fall, or to which only NA values in y were assigned). By default (i.e. if not specified), NA is assigned to such bins.
sortedX	Whether x is sorted.
shiftByHalfBinSize	Logical specifying whether the bins should be shifted by half the bin size to the left. Thus, the first bin will have its center at fromX and its lower and upper boundary are fromX - binSize/2 and fromX + binSize/2. This argument is ignored if breaks are provided.

returnIndex — Logical indicating whether the index of the max (if method = "max") or min (if method = "min") value within each bin in input vector x should also be reported. For methods other than "max" or "min" this argument is ignored.

returnX — logical allowing to avoid returning $x, i.e. the mid-points of the bins. returnX = FALSE might be useful in cases where breaks are pre-defined as it considerably reduces the memory demand.

Details

The breaks defining the boundary of each bin can be either passed directly to the function with the argument breaks, or are calculated on the data based on arguments nBins or binSize along with fromIdx, toIdx and optionally binFromX and binToX. Arguments fromIdx and toIdx allow to specify subset(s) of the input vector x on which bins should be calculated. The default the full x vector is considered. Also, if not specified otherwise with arguments binFromX and binToX , the range of the bins within each of the sub-sets will be from x[fromIdx] to x[toIdx]. Arguments binFromX and binToX allow to overwrite this by manually defining the a range on which the breaks should be calculated. See examples below for more details.

Calculation of breaks: for nBins the breaks correspond to seq(min(x[fromIdx])), max(x[fromIdx], length.out = For binSize the breaks correspond to seq(min(x[fromIdx]), max(x[toIdx]), by = binSize) with the exception that the last break value is forced to be equal to max(x[toIdx]). This ensures that all values from the specified range are covered by the breaks defining the bins. The last bin could however in some instances be slightly larger than binSize. See breaks_on_binSize and breaks_on_nBins for more details.

Value

Returns a list of length 2, the first element (named "x") contains the bin mid-points, the second element (named "y") the aggregated values from input vector y within each bin. For returnIndex = TRUE the list contains an additional element "index" with the index of the max or min (depending on whether method = "max" or method = "min") value within each bin in input vector x.

Note

The function ensures that all values within the range used to define the breaks are considered in the binning (and assigned to a bin). This means that for all bins except the last one values in x have to be >= xlower and < xupper (with xlower and xupper being the lower and upper boundary, respectively). For the last bin the condition is x >= xlower & x <= xupper. Note also that if shiftByHalfBinSize is TRUE the range of values that is used for binning is expanded by binSize (i.e. the lower boundary will be fromX - binSize/2, the upper toX + binSize/2). Setting this argument to TRUE resembles the binning that is/was used in profBin function from xcms < 1.51.

NA handling: by default the function ignores NA values in y (thus inherently assumes na.rm = TRUE). No NA values are allowed in x.

Author(s)

Johannes Rainer

See Also

imputeLinInterpol

Examples

```
########
## Simple example illustrating the breaks and the binning.
##
## Define breaks for 5 bins:
brks <- seq(2, 12, length.out = 6)
## The first bin is then [2,4), the second [4,6) and so on.
brks
## Get the max value falling within each bin.
binYonX(x = 1:16, y = 1:16, breaks = brks)
## Thus, the largest value in x = 1:16 falling into the bin [2,4) (i.e. being
## >= 2 and < 4) is 3, the largest one falling into [4,6) is 5 and so on.
## Note however the function ensures that the minimal and maximal x-value
## (in this example 1 and 12) fall within a bin, i.e. 12 is considered for
## the last bin.

#######
## Performing the binning ons sub-set of x
##
X <- 1:16
## Bin X from element 4 to 10 into 5 bins.
X[4:10]
binYonX(X, X, nBins = 5L, fromIdx = 4, toIdx = 10)
## This defines breaks for 5 bins on the values from 4 to 10 and bins
## the values into these 5 bins. Alternatively, we could manually specify
## the range for the binning, i.e. the minimal and maximal value for the
## breaks:
binYonX(X, X, nBins = 5L, fromIdx = 4, toIdx = 10, binFromX = 1, binToX = 16)
## In this case the breaks for 5 bins were defined from a value 1 to 16 and
## the values 4 to 10 were binned based on these breaks.

#######
## Bin values within a sub-set of x, second example
##
## This example illustrates how the fromIdx and toIdx parameters can be used.
## x defines 3 times the sequence form 1 to 10, while y is the sequence from
## 1 to 30. In this very simple example x is supposed to represent M/Z values
## from 3 consecutive scans and y the intensities measured for each M/Z in
## each scan. We want to get the maximum intensities for M/Z value bins only
## for the second scan, and thus we use fromIdx = 11 and toIdx = 20. The breaks
## for the bins are defined with the nBins, binFromX and binToX.
X <- rep(1:10, 3)
Y <- 1:30
## Bin the M/Z values in the second scan into 5 bins and get the maximum
## intensity for each bin. Note that we have to specify sortedX = TRUE as
## the x and y vectors would be sorted otherwise.
binYonX(X, Y, nBins = 5L, sortedX = TRUE, fromIdx = 11, toIdx = 20)

#######
## Bin in overlapping sub-sets of X
##
## In this example we define overlapping sub-sets of X and perform the binning
## within these.
X <- 1:30
## Define the start and end indices of the sub-sets.
fIdx <- c(2, 8, 21)
```

```
tIdx <- c(10, 25, 30)
binYonX(X, nBins = 5L, fromIdx = fIdx, toIdx = tIdx)
## The same, but pre-defining also the desired range of the bins.
binYonX(X, nBins = 5L, fromIdx = fIdx, toIdx = tIdx, binFromX = 4, binToX = 28)
## The same bins are thus used for each sub-set.
```

`breaks_on_binSize` *Generate breaks for binning using a defined bin size.*

Description

Defines breaks for `binSize` sized bins for values ranging from `fromX` to `toX`.

Usage

```
breaks_on_binSize(fromX, toX, binSize)
```

Arguments

`fromX`	numeric(1) specifying the lowest value for the bins.
`toX`	numeric(1) specifying the largest value for the bins.
`binSize`	numeric(1) defining the size of a bin.

Details

This function creates breaks for bins of size `binSize`. The function ensures that the full data range is included in the bins, i.e. the last value (upper boundary of the last bin) is always equal `toX`. This however means that the size of the last bin will not always be equal to the desired bin size. See examples for more details and a comparisom to R's `seq` function.

Value

A numeric vector defining the lower and upper bounds of the bins.

Author(s)

Johannes Rainer

See Also

`binYonX` for a binning function.

Other functions to define bins: `breaks_on_nBins`

Examples

```
## Define breaks with a size of 0.13 for a data range from 1 to 10:
breaks_on_binSize(1, 10, 0.13)
## The size of the last bin is however larger than 0.13:
diff(breaks_on_binSize(1, 10, 0.13))
## If we would use seq, the max value would not be included:
seq(1, 10, by = 0.13)
```

```
## In the next example we use binSize that leads to an additional last bin with
## a smaller binSize:
breaks_on_binSize(1, 10, 0.51)
## Again, the max value is included, but the size of the last bin is < 0.51.
diff(breaks_on_binSize(1, 10, 0.51))
## Using just seq would result in the following bin definition:
seq(1, 10, by = 0.51)
## Thus it defines one bin (break) less.
```

`breaks_on_nBins` *Generate breaks for binning*

Description

Calculate breaks for same-sized bins for data values from `fromX` to `toX`.

Usage

```
breaks_on_nBins(fromX, toX, nBins, shiftByHalfBinSize = FALSE)
```

Arguments

`fromX`	numeric(1) specifying the lowest value for the bins.
`toX`	numeric(1) specifying the largest value for the bins.
`nBins`	numeric(1) defining the number of bins.
`shiftByHalfBinSize`	Logical indicating whether the bins should be shifted left by half bin size. This results centered bins, i.e. the first bin being centered at `fromX` and the last around `toX`.

Details

This generates bins such as a call to `seq(fromX, toX, length.out = nBins)` would. The first and second element in the result vector thus defines the lower and upper boundary for the first bin, the second and third value for the second bin and so on.

Value

A numeric vector of length `nBins + 1` defining the lower and upper bounds of the bins.

Author(s)

Johannes Rainer

See Also

`binYonX` for a binning function.

Other functions to define bins: `breaks_on_binSize`

Examples

```
## Create breaks to bin values from 3 to 20 into 20 bins
breaks_on_nBins(3, 20, nBins = 20)
## The same call but using shiftByHalfBinSize
breaks_on_nBins(3, 20, nBins = 20, shiftByHalfBinSize = TRUE)
```

---

c-methods *Combine xcmsSet objects*

Description

Combines the samples and peaks from multiple `xcmsSet` objects into a single object. Group and retention time correction data are discarded. The `profinfo` list is set to be equal to the first object.

Arguments

`xs1`	`xcmsSet` object
`...`	`xcmsSet` objects

Value

A `xcmsSet` object.

Methods

xs1 = "xcmsRaw" `c(xs1, ...)`

Author(s)

Colin A. Smith, <csmith@scripps.edu>

See Also

xcmsSet-class

CalibrantMassParam-class *Calibrant mass based calibration of chromatgraphic peaks*

Description

Calibrate peaks using mz values of known masses/calibrants. mz values of identified peaks are adjusted based on peaks that are close to the provided mz values. See details below for more information.

The `isCalibrated` function returns `TRUE` if chromatographic peaks of the XCMSnExp object `x` were calibrated and `FALSE` otherwise.

Usage

```
CalibrantMassParam(mz = list(), mzabs = 1e-04, mzppm = 5, neighbors = 3,
  method = "linear")

isCalibrated(object)

## S4 method for signature 'XCMSnExp'
calibrate(object, param)
```

Arguments

mz	a numeric or list of numeric vectors with reference mz values. If a numeric vector is provided, this is used for each sample in the XCMSnExp object. If a list is provided, it's length has to be equal to the number of samples in the experiment.
mzabs	numeric(1) the absolute error/deviation for matching peaks to calibrants (in Da).
mzppm	numeric(1) the relative error for matching peaks to calibrants in ppm (parts per million).
neighbors	integer(1) with the maximal number of peaks within the permitted distance to the calibrants that are considered. Among these the mz value of the peak with the largest intensity is used in the calibration function estimation.
method	character(1) defining the method that should be used to estimate the calibration function. Can be "shift", "linear" (default) or "edgeshift".
object	An XCMSnExp object.
param	The CalibrantMassParam object with the calibration settings.

Details

The method does first identify peaks that are close to the provided mz values and, given that there difference to the calibrants is smaller than the user provided cut off (based on arguments mzabs and mzppm), their mz values are replaced with the provided mz values. The mz values of all other peaks are either globally shifted (for method = "shift" or estimated by a linear model through all calibrants. Peaks are considered close to a calibrant mz if the difference between the calibrant and its mz is <= mzabs + mz * mzppm /1e6.

Adjustment methods: adjustment function/factor is estimated using the difference between calibrant and peak mz values only for peaks that are close enough to the calibrants. The availabel methods are:

- shift: shifts the m/z of each peak by a global factor which corresponds to the average difference between peak mz and calibrant mz.
- linear: fits a linear model throught the differences between calibrant and peak mz values and adjusts the mz values of all peaks using this.
- edgeshift: performs same adjustment as linear for peaks that are within the mz range of the calibrants and shift outside of it.

For more information, details and examples refer to the *xcms-direct-injection* vignette.

Value

For `CalibrantMassParam`: a `CalibrantMassParam` instance. For `calibrate`: an XCMSnExp object with chromatographic peaks being calibrated. **Be aware** that the actual raw mz values are not (yet) calibrated, but **only** the identified chromatographic peaks.

The `CalibrantMassParam` function returns an instance of the `CalibrantMassParam` class with all settings and properties set.

The `calibrate` method returns an XCMSnExp object with the chromatographic peaks being calibrated. Note that **only** the detected peaks are calibrated, but not the individual mz values in each spectrum.

Note

`CalibrantMassParam` classes don't have exported getter or setter methods.

Author(s)

Joachim Bargsten, Johannes Rainer

`calibrate-methods` *Calibrate peaks for correcting unprecise m/z values*

Description

Calibrate peaks of a xcmsSet via a set of known masses

Arguments

`object`	a `xcmsSet` object with uncalibrated mz
`calibrants`	a vector or a list of vectors with reference m/z-values
`method`	the used calibrating-method, see below
`mzppm`	the relative error used for matching peaks in ppm (parts per million)
`mzabs`	the absolute error used for matching peaks in Da
`neighbours`	the number of neighbours from wich the one with the highest intensity is used (instead of the nearest)
`plotres`	can be set to TRUE if wanted a result-plot showing the found m/z with the distances and the regression

Value

`object`	a `xcmsSet` with one ore more samples
`calibrants`	for each sample different calibrants can be used, if a list of m/z-vectors is given. The length of the list must be the same as the number of samples, alternatively a single vector of masses can be given which is used for all samples.
`method`	"shift" for shifting each m/z, "linear" does a linear regression and adds a linear term to each m/z. "edgeshift" does a linear regression within the range of the mz-calibrants and a shift outside.

Methods

object = "xcmsSet" `calibrate(object, calibrants,method="linear", mzabs=0.0001, mzppm=5, n`

See Also

xcmsSet-class,

---

chromatogram,XCMSnExp-method

Extracting chromatograms

Description

chromatogram: the method allows to extract chromatograms from OnDiskMSnExp and XCMSnExp objects. See also the chromatogram implementation for OnDiskMSnExp in the MSnbase package.

Usage

```
## S4 method for signature 'XCMSnExp'
chromatogram(object, rt, mz, aggregationFun = "sum",
  missing = NA_real_, msLevel = 1L, BPPARAM = bpparam(),
  adjustedRtime = hasAdjustedRtime(object))
```

Arguments

object	Either a OnDiskMSnExp or XCMSnExp object from which the chromatograms should be extracted.
rt	numeric(2) or two-column matrix defining the lower and upper boundary for the retention time range(s). If not specified, the full retention time range of the original data will be used. It is also possible to submit a numeric(1) in which case range is called on it to transform it to a numeric(2).
mz	numeric(2) or two-column matrix defining the lower and upper mz value for the MS data slice(s). If not specified, the chromatograms will be calculated on the full mz range. It is also possible to submit a numeric(1) in which case range is called on it to transform it to a numeric(2).
aggregationFun	character specifying the function to be used to aggregate intensity values across the mz value range for the same retention time. Allowed values are "sum", "max", "mean" and "min".
missing	numeric(1) allowing to specify the intensity value to be used if for a given retention time no signal was measured within the mz range of the corresponding scan. Defaults to NA_real_ (see also Details and Notes sections below). Use missing = 0 to resemble the behaviour of the getEIC from the old user interface.
msLevel	integer specifying the MS level from which the chromatogram should be extracted. Defaults to msLevel = 1L.
BPPARAM	Parallelisation backend to be used, which will depend on the architecture. Default is BiocParallel::bparam().

adjustedRtime For chromatogram,XCMSnExp: whether the adjusted (adjustedRtime = TRUE) or raw retention times (adjustedRtime = FALSE) should be used for filtering and returned in the resulting Chromatogram object. Adjusted retention times are used by default if available.

Details

Arguments rt and mz allow to specify the MS data slice from which the chromatogram should be extracted. The parameter aggregationSum allows to specify the function to be used to aggregate the intensities across the mz range for the same retention time. Setting aggregationFun = "sum" would e.g. allow to calculate the *total ion chromatogram* (TIC), aggregationFun = "max" the *base peak chromatogram* (BPC). The length of the extracted Chromatogram object, i.e. the number of available data points, corresponds to the number of scans/spectra measured in the specified retention time range. If in a specific scan (for a give retention time) no signal was measured in the specified mz range, a NA_real_ is reported as intensity for the retention time (see Notes for more information). This can be changed using the missing parameter.

Value

chromatogram returns a Chromatograms object with the number of columns corresponding to the number of files in object and number of rows the number of specified ranges (i.e. number of rows of matrices provided with arguments mz and/or rt).

Note

Chromatogram objects extracted with chromatogram contain NA_real_ values if, for a given retention time, no signal was measured in the specified mz range. If no spectrum/scan is present in the defined retention time window a Chromatogram object of length 0 is returned.

For XCMSnExp objects, if adjusted retention times are available, the chromatogram method will by default report and use these (for the subsetting based on the provided parameter rt). This can be overwritten with the parameter adjustedRtime.

Author(s)

Johannes Rainer

See Also

XCMSnExp for the data object. Chromatogram for the object representing chromatographic data.

Chromatograms for the object allowing to arrange multiple Chromatogram objects.

plot to plot a Chromatogram or Chromatograms objects.

extractMsData for a method to extract the MS data as data.frame.

Examples

```
## Read some files from the faahKO package.
library(xcms)
library(faahKO)
faahko_3_files <- c(system.file('cdf/KO/ko15.CDF', package = "faahKO"),
                    system.file('cdf/KO/ko16.CDF', package = "faahKO"),
                    system.file('cdf/KO/ko18.CDF', package = "faahKO"))

od <- readMSData(faahko_3_files, mode = "onDisk")
```

```
## Extract the ion chromatogram for one chromatographic peak in the data.
chrs <- chromatogram(od, rt = c(2700, 2900), mz = 335)

chrs

## Plot the chromatogram
plot(rtime(chrs[1, 2]), intensity(chrs[1, 2]), type = "l", xlab = "rtime",
     ylab = "intensity", col = "000080")
for(i in c(1, 3)) {
  points(rtime(chrs[1, i]), intensity(chrs[1, i]), type = "l",
  col = "00000080")
}

## Plot the chromatogram using the dedicated plot method.
plot(chrs)

## Extract chromatograms for multiple ranges.
mzr <- matrix(c(335, 335, 344, 344), ncol = 2, byrow = TRUE)
rtr <- matrix(c(2700, 2900, 2600, 2750), ncol = 2, byrow = TRUE)
chrs <- chromatogram(od, mz = mzr, rt = rtr)

chrs

## Plot the extracted chromatograms
plot(chrs)

## Get access to all chromatograms for the second mz/rt range
chrs[1, ]

## Plot just that one
plot(chrs[1, , drop = FALSE])
```

`chromatographic-peak-detection` *Chromatographic peak detection methods.*

Description

The `findChromPeaks` methods perform the chromatographic peak detection on LC/GC-MS data and are part of the modernized `xcms` user interface.

The implemented peak detection methods in chromatographic space are:

centWave chromatographic peak detection using the *centWave* method. See `centWave` for more details.

centWave with predicted isotopes peak detection using a two-step centWave-based approach considering also feature isotopes. See `centWaveWithPredIsoROIs` for more details.

matchedFilter peak detection in chromatographic space. See `matchedFilter` for more details.

massifquant peak detection using the Kalman filter-based method. See `massifquant` for more details.

MSW single-spectrum non-chromatography MS data peak detection. See `MSW` for more details.

Author(s)

Johannes Rainer

See Also

`findPeaks` for the *old* peak detection methods.

`plotChromPeaks` to plot identified chromatographic peaks for one file.

`highlightChromPeaks` to highlight identified chromatographic peaks in an extracted ion chromatogram plot.

Other peak detection methods: `findChromPeaks-centWaveWithPredIsoROIs`, `findChromPeaks-centWave`, `findChromPeaks-massifquant`, `findChromPeaks-matchedFilter`, `findPeaks-MSW`

---

collect-methods *Collect MS^n peaks into xcmsFragments*

Description

Collecting Peaks into `xcmsFragments`s from several MS-runs using `xcmsSet` and `xcmsRaw`.

Arguments

`object`	(empty) `xcmsFragments-class` object
`xs`	A `xcmsSet-class` object which contains picked ms1-peaks from several experiments
`compMethod`	("floor", "round", "none"): compare-method which is used to find the parent peak of a MSnpeak through comparing the MZ-values of the MS1peaks with the MSnParentPeaks.
`snthresh, mzgap, uniq`	these are the parameters for the getspec-peakpicker included in xcmsRaw.

Details

After running collect(xFragments,xSet) The peak table of the xcmsFragments includes the ms1Peaks from all experiments stored in a xcmsSet-object. Further it contains the relevant msN-peaks from the xcmsRaw-objects, which were created temporarily with the paths in xcmsSet.

Value

A matrix with columns:

`peakID`	unique identifier of every peak
`MSnParentPeakID`	PeakID of the parent peak of a msLevel>1 - peak, it is 0 if the peak is msLevel 1.
`msLevel`	The msLevel of the peak.
`rt`	retention time of the peak midpoint
`mz`	the mz-Value of the peak
`intensity`	the intensity of the peak

sample	the number of the sample from the xcmsSet
GroupPeakMSn	Used for grouped xcmsSet groups
CollisionEnergy	The collision energy of the fragment

Methods

object = "xcmsFragments" collect(object, ...)

---

diffreport-methods *Create report of analyte differences*

Description

Create a report showing the most significant differences between two sets of samples. Optionally create extracted ion chromatograms for the most significant differences.

Arguments

object	the xcmsSet object
class1	character vector with the first set of sample classes to be compared
class2	character vector with the second set of sample classes to be compared
filebase	base file name to save report, .tsv file and _eic will be appended to this name for the tabular report and EIC directory, respectively. if blank nothing will be saved
eicmax	number of the most significantly different analytes to create EICs for
eicwidth	width (in seconds) of EICs produced
sortpval	logical indicating whether the reports should be sorted by p-value
classeic	character vector with the sample classes to include in the EICs
value	intensity values to be used for the diffreport. If value="into", integrated peak intensities are used. If value="maxo", maximum peak intensities are used. If value="intb", baseline corrected integrated peak intensities are used (only available if peak detection was done by findPeaks.centWave).
metlin	mass uncertainty to use for generating link to Metlin metabolite database. the sign of the uncertainty indicates negative or positive mode data for M+H or M-H calculation. a value of FALSE or 0 removes the column
h	Numeric variable for the height of the eic and boxplots that are printed out.
w	Numeric variable for the width of the eic and boxplots print out made.
mzdec	Number of decimal places of title m/z values in the eic plot.
...	optional arguments to be passed to mt.teststat

Details

This method handles creation of summary reports with statistics about which analytes were most significantly different between two sets of samples. It computes Welch's two-sample t-statistic for each analyte and ranks them by p-value. It returns a summary report that can optionally be written out to a tab-separated file.

Additionally, it does all the heavy lifting involved in creating superimposed extracted ion chromatograms for a given number of analytes. It does so by reading the raw data files associated with the samples of interest one at a time. As it does so, it prints the name of the sample it is currently reading. Depending on the number and size of the samples, this process can take a long time.

If a base file name is provided, the report (see Value section) will be saved to a tab separated file. If EICs are generated, they will be saved as 640x480 PNG files in a newly created subdirectory. However this parameter can be changed with the commands arguments. The numbered file names correspond to the rows in the report.

Chromatographic traces in the EICs are colored and labeled by their sample class. Sample classes take their color from the current palette. The color a sample class is assigned is dependent its order in the `xcmsSet` object, not the order given in the class arguments. Thus `levels(sampclass(object))[1]` would use color `palette()[1]` and so on. In that way, sample classes maintain the same color across any number of different generated reports.

When there are multiple sample classes, xcms will produce boxplots of the different classes and will generate a single anova p-value statistic. Like the eic's the plot number corresponds to the row number in the report.

Value

A data frame with the following columns:

`fold`	mean fold change (always greater than 1, see `tstat` for which set of sample classes was higher)
`tstat`	Welch's two sample t-statistic, positive for analytes having greater intensity in `class2`, negative for analytes having greater intensity in `class1`
`pvalue`	p-value of t-statistic
`anova`	p-value of the anova statistic if there are multiple classes
`mzmed`	median m/z of peaks in the group
`mzmin`	minimum m/z of peaks in the group
`mzmax`	maximum m/z of peaks in the group
`rtmed`	median retention time of peaks in the group
`rtmin`	minimum retention time of peaks in the group
`rtmax`	maximum retention time of peaks in the group
`npeaks`	number of peaks assigned to the group
`Sample Classes`	number samples from each sample class represented in the group
`metlin`	A URL to metlin for that mass
`...`	one column for every sample class
`Sample Names`	integrated intensity value for every sample
`...`	one column for every sample

Methods

object = "xcmsSet" `diffreport(object, class1 = levels(sampclass(object))[1],` `class2`

See Also

xcmsSet-class, mt.teststat, palette

---

do_adjustRtime_peakGroups *Align spectrum retention times across samples using peak groups found in most samples*

Description

The function performs retention time correction by assessing the retention time deviation across all samples using peak groups (features) containg chromatographic peaks present in most/all samples. The retention time deviation for these features in each sample is described by fitting either a polynomial (`smooth = "loess"`) or a linear (`smooth = "linear"`) model to the data points. The models are subsequently used to adjust the retention time for each spectrum in each sample.

Usage

```
do_adjustRtime_peakGroups(peaks, peakIndex, rtime, minFraction = 0.9,
  extraPeaks = 1, smooth = c("loess", "linear"), span = 0.2,
  family = c("gaussian", "symmetric"), peakGroupsMatrix = matrix(ncol = 0,
  nrow = 0))
```

Arguments

`peaks`	a `matrix` or `data.frame` with the identified chromatographic peaks in the samples.
`peakIndex`	a `list` of indices that provides the grouping information of the chromatographic peaks (across and within samples).
`rtime`	a `list` of `numeric` vectors with the retention times per file/sample.
`minFraction`	`numeric(1)` between 0 and 1 defining the minimum required fraction of samples in which peaks for the peak group were identified. Peak groups passing this criteria will aligned across samples and retention times of individual spectra will be adjusted based on this alignment. For `minFraction = 1` the peak group has to contain peaks in all samples of the experiment.
`extraPeaks`	`numeric(1)` defining the maximal number of additional peaks for all samples to be assigned to a peak group (i.e. feature) for retention time correction. For a data set with 6 samples, `extraPeaks = 1` uses all peak groups with a total peak count `<= 6 + 1`. The total peak count is the total number of peaks being assigned to a peak group and considers also multiple peaks within a sample being assigned to the group.
`smooth`	character defining the function to be used, to interpolate corrected retention times for all peak groups. Either `"loess"` or `"linear"`.
`span`	`numeric(1)` defining the degree of smoothing (if `smooth = "loess"`). This parameter is passed to the internal call to `loess`.
`family`	character defining the method to be used for loess smoothing. Allowed values are `"gaussian"` and `"symmetric"`.See `loess` for more information.

peakGroupsMatrix
: optional matrix of (raw) retention times for peak groups on which the alignment should be performed. Each column represents a sample, each row a feature/peak group. If not provided, this matrix will be determined depending on parameters minFraction and extraPeaks. If provided, minFraction and extraPeaks will be ignored.

Details

The alignment bases on the presence of compounds that can be found in all/most samples of an experiment. The retention times of individual spectra are then adjusted based on the alignment of the features corresponding to these *house keeping compounds*. The paraneters minFraction and extraPeaks can be used to fine tune which features should be used for the alignment (i.e. which features most likely correspond to the above mentioned house keeping compounds).

Value

A list with numeric vectors with the adjusted retention times grouped by sample.

Note

The method ensures that returned adjusted retention times are increasingly ordered, just as the raw retention times.

Author(s)

Colin Smith, Johannes Rainer

References

Colin A. Smith, Elizabeth J. Want, Grace O'Maille, Ruben Abagyan and Gary Siuzdak. "XCMS: Processing Mass Spectrometry Data for Metabolite Profiling Using Nonlinear Peak Alignment, Matching, and Identification" *Anal. Chem.* 2006, 78:779-787.

---

do_findChromPeaks_centWave

Core API function for centWave peak detection

Description

This function performs peak density and wavelet based chromatographic peak detection for high resolution LC/MS data in centroid mode [Tautenhahn 2008].

Usage

```
do_findChromPeaks_centWave(mz, int, scantime, valsPerSpect, ppm = 25,
  peakwidth = c(20, 50), snthresh = 10, prefilter = c(3, 100),
  mzCenterFun = "wMean", integrate = 1, mzdiff = -0.001,
  fitgauss = FALSE, noise = 0, verboseColumns = FALSE, roiList = list(),
  firstBaselineCheck = TRUE, roiScales = NULL, sleep = 0)
```

Arguments

mz	Numeric vector with the individual m/z values from all scans/ spectra of one file/sample.
int	Numeric vector with the individual intensity values from all scans/spectra of one file/sample.
scantime	Numeric vector of length equal to the number of spectra/scans of the data representing the retention time of each scan.
valsPerSpect	Numeric vector with the number of values for each spectrum.
ppm	numeric(1) defining the maximal tolerated m/z deviation in consecutive scans in parts per million (ppm) for the initial ROI definition.
peakwidth	numeric(2) with the expected approximate peak width in chromatographic space. Given as a range (min, max) in seconds.
snthresh	numeric(1) defining the signal to noise ratio cutoff.
prefilter	numeric(2): c(k, I) specifying the prefilter step for the first analysis step (ROI detection). Mass traces are only retained if they contain at least k peaks with intensity >= I.
mzCenterFun	Name of the function to calculate the m/z center of the chromatographic peak. Allowed are: "wMean": intensity weighted mean of the peak's m/z values, "mean": mean of the peak's m/z values, "apex": use the m/z value at the peak apex, "wMeanApex3": intensity weighted mean of the m/z value at the peak apex and the m/z values left and right of it and "meanApex3": mean of the m/z value of the peak apex and the m/z values left and right of it.
integrate	Integration method. For integrate = 1 peak limits are found through descent on the mexican hat filtered data, for integrate = 2 the descent is done on the real data. The latter method is more accurate but prone to noise, while the former is more robust, but less exact.
mzdiff	numeric(1) representing the minimum difference in m/z dimension for peaks with overlapping retention times; can be negatove to allow overlap.
fitgauss	logical(1) whether or not a Gaussian should be fitted to each peak.
noise	numeric(1) allowing to set a minimum intensity required for centroids to be considered in the first analysis step (centroids with intensity < noise are omitted from ROI detection).
verboseColumns	logical(1) whether additional peak meta data columns should be returned.
roiList	An optional list of regions-of-interest (ROI) representing detected mass traces. If ROIs are submitted the first analysis step is omitted and chromatographic peak detection is performed on the submitted ROIs. Each ROI is expected to have the following elements specified: scmin (start scan index), scmax (end scan index), mzmin (minimum m/z), mzmax (maximum m/z), length (number of scans), intensity (summed intensity). Each ROI should be represented by a list of elements or a single row data.frame.
firstBaselineCheck	logical(1). If TRUE continuous data within regions of interest is checked to be above the first baseline.
roiScales	Optional numeric vector with length equal to roiList defining the scale for each region of interest in roiList that should be used for the centWave-wavelets.
sleep	numeric(1) defining the number of seconds to wait between iterations. Defaults to sleep = 0. If > 0 a plot is generated visualizing the identified chromatographic peak. Note: this argument is for backward compatibility only and will be removed in future.

Details

This algorithm is most suitable for high resolution LC/{TOF,OrbiTrap,FTICR}-MS data in centroid mode. In the first phase the method identifies *regions of interest* (ROIs) representing mass traces that are characterized as regions with less than ppm m/z deviation in consecutive scans in the LC/MS map. These ROIs are then subsequently analyzed using continuous wavelet transform (CWT) to locate chromatographic peaks on different scales. The first analysis step is skipped, if regions of interest are passed with the `roiList` parameter.

Value

A matrix, each row representing an identified chromatographic peak, with columns:

mz Intensity weighted mean of m/z values of the peak across scans.

mzmin Minimum m/z of the peak.

mzmax Maximum m/z of the peak.

rt Retention time of the peak's midpoint.

rtmin Minimum retention time of the peak.

rtmax Maximum retention time of the peak.

into Integrated (original) intensity of the peak.

intb Per-peak baseline corrected integrated peak intensity.

maxo Maximum intensity of the peak.

sn Signal to noise ratio, defined as `(maxo - baseline)/sd`, `sd` being the standard deviation of local chromatographic noise.

egauss RMSE of Gaussian fit.

Additional columns for `verboseColumns = TRUE`:

mu Gaussian parameter mu.

sigma Gaussian parameter sigma.

h Gaussian parameter h.

f Region number of the m/z ROI where the peak was localized.

dppm m/z deviation of mass trace across scans in ppm.

scale Scale on which the peak was localized.

scpos Peak position found by wavelet analysis (scan number).

scmin Left peak limit found by wavelet analysis (scan number).

scmax Right peak limit found by wavelet analysis (scan numer).

Note

The *centWave* was designed to work on centroided mode, thus it is expected that such data is presented to the function.

This function exposes core chromatographic peak detection functionality of the *centWave* method. While this function can be called directly, users will generally call the corresponding method for the data object instead.

Author(s)

Ralf Tautenhahn, Johannes Rainer

References

Ralf Tautenhahn, Christoph B\"ottcher, and Steffen Neumann "Highly sensitive feature detection for high resolution LC/MS" *BMC Bioinformatics* 2008, 9:504

See Also

centWave for the standard user interface method.

Other core peak detection functions: do_findChromPeaks_centWaveWithPredIsoROIs, do_findChromPeaks_massifc
do_findChromPeaks_matchedFilter, do_findPeaks_MSW

Examples

```
## Load the test file
library(faahKO)
fs <- system.file('cdf/KO/ko15.CDF', package = "faahKO")
xr <- xcmsRaw(fs, profstep = 0)

## Extracting the data from the xcmsRaw for do_findChromPeaks_centWave
mzVals <- xr@env$mz
intVals <- xr@env$intensity
## Define the values per spectrum:
valsPerSpect <- diff(c(xr@scanindex, length(mzVals)))

## Calling the function. We're using a large value for noise to speed up
## the call in the example performance - in a real use case we would either
## set the value to a reasonable value or use the default value.
res <- do_findChromPeaks_centWave(mz = mzVals, int = intVals,
scantime = xr@scantime, valsPerSpect = valsPerSpect, noise = 10000)
head(res)
```

---

do_findChromPeaks_centWaveWithPredIsoROIs

Core API function for two-step centWave peak detection with isotopes

---

Description

The do_findChromPeaks_centWaveWithPredIsoROIs performs a two-step centWave based peak detection: chromatographic peaks are identified using centWave followed by a prediction of the location of the identified peaks' isotopes in the mz-retention time space. These locations are fed as *regions of interest* (ROIs) to a subsequent centWave run. All non overlapping peaks from these two peak detection runs are reported as the final list of identified peaks.

The do_findChromPeaks_centWaveAddPredIsoROIs performs centWave based peak detection based in regions of interest (ROIs) representing predicted isotopes for the peaks submitted with argument peaks.. The function returns a matrix with the identified peaks consisting of all input peaks and peaks representing predicted isotopes of these (if found by the centWave algorithm).

Usage

```
do_findChromPeaks_centWaveWithPredIsoROIs(mz, int, scantime, valsPerSpect,
  ppm = 25, peakwidth = c(20, 50), snthresh = 10, prefilter = c(3, 100),
  mzCenterFun = "wMean", integrate = 1, mzdiff = -0.001,
```

```
  fitgauss = FALSE, noise = 0, verboseColumns = FALSE, roiList = list(),
  firstBaselineCheck = TRUE, roiScales = NULL, snthreshIsoROIs = 6.25,
  maxCharge = 3, maxIso = 5, mzIntervalExtension = TRUE,
  polarity = "unknown")

do_findChromPeaks_addPredIsoROIs(mz, int, scantime, valsPerSpect, ppm = 25,
  peakwidth = c(20, 50), snthresh = 6.25, prefilter = c(3, 100),
  mzCenterFun = "wMean", integrate = 1, mzdiff = -0.001,
  fitgauss = FALSE, noise = 0, verboseColumns = FALSE, peaks. = NULL,
  maxCharge = 3, maxIso = 5, mzIntervalExtension = TRUE,
  polarity = "unknown")
```

Arguments

mz	Numeric vector with the individual m/z values from all scans/ spectra of one file/sample.
int	Numeric vector with the individual intensity values from all scans/spectra of one file/sample.
scantime	Numeric vector of length equal to the number of spectra/scans of the data representing the retention time of each scan.
valsPerSpect	Numeric vector with the number of values for each spectrum.
ppm	numeric(1) defining the maximal tolerated m/z deviation in consecutive scans in parts per million (ppm) for the initial ROI definition.
peakwidth	numeric(2) with the expected approximate peak width in chromatographic space. Given as a range (min, max) in seconds.
snthresh	For do_findChromPeaks_addPredIsoROIs: numeric(1) defining the signal to noise threshold for the centWave algorithm. For do_findChromPeaks_centWaveWithPredIsoROIs: numeric(1) defining the signal to noise threshold for the initial (first) centWave run.
prefilter	numeric(2): c(k, I) specifying the prefilter step for the first analysis step (ROI detection). Mass traces are only retained if they contain at least k peaks with intensity >= I.
mzCenterFun	Name of the function to calculate the m/z center of the chromatographic peak. Allowed are: "wMean": intensity weighted mean of the peak's m/z values, "mean": mean of the peak's m/z values, "apex": use the m/z value at the peak apex, "wMeanApex3": intensity weighted mean of the m/z value at the peak apex and the m/z values left and right of it and "meanApex3": mean of the m/z value of the peak apex and the m/z values left and right of it.
integrate	Integration method. For integrate = 1 peak limits are found through descent on the mexican hat filtered data, for integrate = 2 the descent is done on the real data. The latter method is more accurate but prone to noise, while the former is more robust, but less exact.
mzdiff	numeric(1) representing the minimum difference in m/z dimension for peaks with overlapping retention times; can be negatove to allow overlap.
fitgauss	logical(1) whether or not a Gaussian should be fitted to each peak.
noise	numeric(1) allowing to set a minimum intensity required for centroids to be considered in the first analysis step (centroids with intensity < noise are omitted from ROI detection).
verboseColumns	logical(1) whether additional peak meta data columns should be returned.

`roiList` An optional list of regions-of-interest (ROI) representing detected mass traces. If ROIs are submitted the first analysis step is omitted and chromatographic peak detection is performed on the submitted ROIs. Each ROI is expected to have the following elements specified: `scmin` (start scan index), `scmax` (end scan index), `mzmin` (minimum m/z), `mzmax` (maximum m/z), `length` (number of scans), `intensity` (summed intensity). Each ROI should be represented by a `list` of elements or a single row `data.frame`.

`firstBaselineCheck` `logical(1)`. If `TRUE` continuous data within regions of interest is checked to be above the first baseline.

`roiScales` Optional numeric vector with length equal to `roiList` defining the scale for each region of interest in `roiList` that should be used for the centWave-wavelets.

`snthreshIsoROIs` `numeric(1)` defining the signal to noise ratio cutoff to be used in the second centWave run to identify peaks for predicted isotope ROIs.

`maxCharge` `integer(1)` defining the maximal isotope charge. Isotopes will be defined for charges `1:maxCharge`.

`maxIso` `integer(1)` defining the number of isotope peaks that should be predicted for each peak identified in the first centWave run.

`mzIntervalExtension` `logical(1)` whether the mz range for the predicted isotope ROIs should be extended to increase detection of low intensity peaks.

`polarity` `character(1)` specifying the polarity of the data. Currently not used, but has to be `"positive"`, `"negative"` or `"unknown"` if provided.

`peaks.` A matrix or `xcmsPeaks` object such as one returned by a call to `link{do_findChromPeaks_centWave` or `link{findPeaks.centWave}` (both with `verboseColumns = TRUE`) with the peaks for which isotopes should be predicted and used for an additional peak detectoin using the centWave method. Required columns are: `"mz"`, `"mzmin"`, `"mzmax"`, `"scmin"`, `"scmax"`, `"scale"` and `"into"`.

Details

For more details on the centWave algorithm see `centWave`.

Value

A matrix, each row representing an identified chromatographic peak. All non-overlapping peaks identified in both centWave runs are reported. The matrix columns are:

mz Intensity weighted mean of m/z values of the peaks across scans.

mzmin Minimum m/z of the peaks.

mzmax Maximum m/z of the peaks.

rt Retention time of the peak's midpoint.

rtmin Minimum retention time of the peak.

rtmax Maximum retention time of the peak.

into Integrated (original) intensity of the peak.

intb Per-peak baseline corrected integrated peak intensity.

maxo Maximum intensity of the peak.

sn Signal to noise ratio, defined as `(maxo - baseline)/sd`, `sd` being the standard deviation of local chromatographic noise.

egauss RMSE of Gaussian fit.

Additional columns for `verboseColumns = TRUE`:

mu Gaussian parameter mu.

sigma Gaussian parameter sigma.

h Gaussian parameter h.

f Region number of the m/z ROI where the peak was localized.

dppm m/z deviation of mass trace across scans in ppm.

scale Scale on which the peak was localized.

scpos Peak position found by wavelet analysis (scan number).

scmin Left peak limit found by wavelet analysis (scan number).

scmax Right peak limit found by wavelet analysis (scan numer).

Author(s)

Hendrik Treutler, Johannes Rainer

See Also

Other core peak detection functions: `do_findChromPeaks_centWave`, `do_findChromPeaks_massifquant`, `do_findChromPeaks_matchedFilter`, `do_findPeaks_MSW`

`do_findChromPeaks_massifquant`
Core API function for massifquant peak detection

Description

Massifquant is a Kalman filter (KF)-based chromatographic peak detection for XC-MS data in centroid mode. The identified peaks can be further refined with the *centWave* method (see `do_findChromPeaks_centWave` for details on centWave) by specifying `withWave = TRUE`.

Usage

```
do_findChromPeaks_massifquant(mz, int, scantime, valsPerSpect, ppm = 10,
  peakwidth = c(20, 50), snthresh = 10, prefilter = c(3, 100),
  mzCenterFun = "wMean", integrate = 1, mzdiff = -0.001,
  fitgauss = FALSE, noise = 0, verboseColumns = FALSE,
  criticalValue = 1.125, consecMissedLimit = 2, unions = 1,
  checkBack = 0, withWave = FALSE)
```

Arguments

mz	Numeric vector with the individual m/z values from all scans/ spectra of one file/sample.
int	Numeric vector with the individual intensity values from all scans/spectra of one file/sample.
scantime	Numeric vector of length equal to the number of spectra/scans of the data representing the retention time of each scan.
valsPerSpect	Numeric vector with the number of values for each spectrum.
ppm	numeric(1) defining the maximal tolerated m/z deviation in consecutive scans in parts per million (ppm) for the initial ROI definition.
peakwidth	numeric(2) with the expected approximate peak width in chromatographic space. Given as a range (min, max) in seconds.
snthresh	numeric(1) defining the signal to noise ratio cutoff.
prefilter	numeric(2): c(k, I) specifying the prefilter step for the first analysis step (ROI detection). Mass traces are only retained if they contain at least k peaks with intensity >= I.
mzCenterFun	Name of the function to calculate the m/z center of the chromatographic peak. Allowed are: "wMean": intensity weighted mean of the peak's m/z values, "mean": mean of the peak's m/z values, "apex": use the m/z value at the peak apex, "wMeanApex3": intensity weighted mean of the m/z value at the peak apex and the m/z values left and right of it and "meanApex3": mean of the m/z value of the peak apex and the m/z values left and right of it.
integrate	Integration method. For integrate = 1 peak limits are found through descent on the mexican hat filtered data, for integrate = 2 the descent is done on the real data. The latter method is more accurate but prone to noise, while the former is more robust, but less exact.
mzdiff	numeric(1) representing the minimum difference in m/z dimension for peaks with overlapping retention times; can be negatove to allow overlap.
fitgauss	logical(1) whether or not a Gaussian should be fitted to each peak.
noise	numeric(1) allowing to set a minimum intensity required for centroids to be considered in the first analysis step (centroids with intensity < noise are omitted from ROI detection).
verboseColumns	logical(1) whether additional peak meta data columns should be returned.
criticalValue	numeric(1). Suggested values: (0.1-3.0). This setting helps determine the the Kalman Filter prediciton margin of error. A real centroid belonging to a bonafide peak must fall within the KF prediction margin of error. Much like in the construction of a confidence interval, criticalVal loosely translates to be a multiplier of the standard error of the prediction reported by the Kalman Filter. If the peak in the XC-MS sample have a small mass deviance in ppm error, a smaller critical value might be better and vice versa.
consecMissedLimit	integer(1) Suggested values: (1,2,3). While a peak is in the proces of being detected by a Kalman Filter, the Kalman Filter may not find a predicted centroid in every scan. After 1 or more consecutive failed predictions, this setting informs Massifquant when to stop a Kalman Filter from following a candidate peak.
unions	integer(1) set to 1 if apply t-test union on segmentation; set to 0 if no t-test to be applied on chromatographically continous peaks sharing same m/z range. Explanation: With very few data points, sometimes a Kalman Filter stops tracking

a peak prematurely. Another Kalman Filter is instantiated and begins following the rest of the signal. Because tracking is done backwards to forwards, this algorithmic defect leaves a real peak divided into two segments or more. With this option turned on, the program identifies segmented peaks and combines them (merges them) into one with a two sample t-test. The potential danger of this option is that some truly distinct peaks may be merged.

`checkBack` `integer(1)` set to `1` if turned on; set to `0` if turned off. The convergence of a Kalman Filter to a peak's precise m/z mapping is very fast, but sometimes it incorporates erroneous centroids as part of a peak (especially early on). The `scanBack` option is an attempt to remove the occasional outlier that lies beyond the converged bounds of the Kalman Filter. The option does not directly affect identification of a peak because it is a postprocessing measure; it has not shown to be a extremely useful thus far and the default is set to being turned off.

`withWave` `logical(1)` if `TRUE`, the peaks identified first with Massifquant are subsequently filtered with the second step of the centWave algorithm, which includes wavelet estimation.

Details

This algorithm's performance has been tested rigorously on high resolution LC/OrbiTrap, TOF-MS data in centroid mode. Simultaneous kalman filters identify peaks and calculate their area under the curve. The default parameters are set to operate on a complex LC-MS Orbitrap sample. Users will find it useful to do some simple exploratory data analysis to find out where to set a minimum intensity, and identify how many scans an average peak spans. The `consecMissedLimit` parameter has yielded good performance on Orbitrap data when set to (`2`) and on TOF data it was found best to be at (`1`). This may change as the algorithm has yet to be tested on many samples. The `criticalValue` parameter is perhaps most dificult to dial in appropriately and visual inspection of peak identification is the best suggested tool for quick optimization. The `ppm` and `checkBack` parameters have shown less influence than the other parameters and exist to give users flexibility and better accuracy.

Value

A matrix, each row representing an identified chromatographic peak, with columns:

mz Intensity weighted mean of m/z values of the peaks across scans.

mzmin Minumum m/z of the peak.

mzmax Maximum m/z of the peak.

rtmin Minimum retention time of the peak.

rtmax Maximum retention time of the peak.

rt Retention time of the peak's midpoint.

into Integrated (original) intensity of the peak.

maxo Maximum intensity of the peak.

If `withWave` is set to `TRUE`, the result is the same as returned by the `do_findChromPeaks_centWave` method.

Author(s)

Christopher Conley

References

Conley CJ, Smith R, Torgrip RJ, Taylor RM, Tautenhahn R and Prince JT "Massifquant: open-source Kalman filter-based XC-MS isotope trace feature detection" *Bioinformatics* 2014, 30(18):2636-43.

See Also

`massifquant` for the standard user interface method.

Other core peak detection functions: `do_findChromPeaks_centWaveWithPredIsoROIs`, `do_findChromPeaks_centWav`
`do_findChromPeaks_matchedFilter`, `do_findPeaks_MSW`

Examples

```
library(faahKO)
library(xcms)
cdfpath <- system.file("cdf", package = "faahKO")
cdffiles <- list.files(cdfpath, recursive = TRUE, full.names = TRUE)

## Read the first file
xraw <- xcmsRaw(cdffiles[1])
## Extract the required data
mzVals <- xraw@env$mz
intVals <- xraw@env$intensity
## Define the values per spectrum:
valsPerSpect <- diff(c(xraw@scanindex, length(mzVals)))

## Perform the peak detection using massifquant
res <- do_findChromPeaks_massifquant(mz = mzVals, int = intVals,
scantime = xraw@scantime, valsPerSpect = valsPerSpect)
head(res)
```

---

do_findChromPeaks_matchedFilter

Core API function for matchedFilter peak detection

Description

This function identifies peaks in the chromatographic time domain as described in [Smith 2006]. The intensity values are binned by cutting The LC/MS data into slices (bins) of a mass unit (`binSize` m/z) wide. Within each bin the maximal intensity is selected. The peak detection is then performed in each bin by extending it based on the `steps` parameter to generate slices comprising bins `current_bin - steps +1` to `current_bin + steps - 1`. Each of these slices is then filtered with matched filtration using a second-derative Gaussian as the model peak shape. After filtration peaks are detected using a signal-to-ration cut-off. For more details and illustrations see [Smith 2006].

Usage

```
do_findChromPeaks_matchedFilter(mz, int, scantime, valsPerSpect,
  binSize = 0.1, impute = "none", baseValue, distance, fwhm = 30,
  sigma = fwhm/2.3548, max = 5, snthresh = 10, steps = 2, mzdiff = 0.8
  - binSize * steps, index = FALSE, sleep = 0)
```

Arguments

mz	Numeric vector with the individual m/z values from all scans/ spectra of one file/sample.
int	Numeric vector with the individual intensity values from all scans/spectra of one file/sample.
scantime	Numeric vector of length equal to the number of spectra/scans of the data representing the retention time of each scan.
valsPerSpect	Numeric vector with the number of values for each spectrum.
binSize	numeric(1) specifying the width of the bins/slices in m/z dimension.
impute	Character string specifying the method to be used for missing value imputation. Allowed values are "none" (no linear interpolation), "lin" (linear interpolation), "linbase" (linear interpolation within a certain bin-neighborhood) and "intlin". See imputeLinInterpol for more details.
baseValue	The base value to which empty elements should be set. This is only considered for method = "linbase" and corresponds to the profBinLinBase's baselevel argument.
distance	For method = "linbase": number of non-empty neighboring element of an empty element that should be considered for linear interpolation. See details section for more information.
fwhm	numeric(1) specifying the full width at half maximum of matched filtration gaussian model peak. Only used to calculate the actual sigma, see below.
sigma	numeric(1) specifying the standard deviation (width) of the matched filtration model peak.
max	numeric(1) representing the maximum number of peaks that are expected/will be identified per slice.
snthresh	numeric(1) defining the signal to noise ratio cutoff.
steps	numeric(1) defining the number of bins to be merged before filtration (i.e. the number of neighboring bins that will be joined to the slice in which filtration and peak detection will be performed).
mzdiff	numeric(1) representing the minimum difference in m/z dimension for peaks with overlapping retention times; can be negatove to allow overlap.
index	logical(1) specifying whether indicies should be returned instead of values for m/z and retention times.
sleep	numeric(1) defining the number of seconds to wait between iterations. Defaults to sleep = 0. If > 0 a plot is generated visualizing the identified chromatographic peak. Note: this argument is for backward compatibility only and will be removed in future.

Details

The intensities are binned by the provided m/z values within each spectrum (scan). Binning is performed such that the bins are centered around the m/z values (i.e. the first bin includes all m/z values between min(mz) - bin_size/2 and min(mz) + bin_size/2).

For more details on binning and missing value imputation see binYonX and imputeLinInterpol methods.

Value

A matrix, each row representing an identified chromatographic peak, with columns:

mz Intensity weighted mean of m/z values of the peak across scans.

mzmin Minimum m/z of the peak.

mzmax Maximum m/z of the peak.

rt Retention time of the peak's midpoint.

rtmin Minimum retention time of the peak.

rtmax Maximum retention time of the peak.

into Integrated (original) intensity of the peak.

intf Integrated intensity of the filtered peak.

maxo Maximum intensity of the peak.

maxf Maximum intensity of the filtered peak.

i Rank of peak in merged EIC (`<= max`).

sn Signal to noise ratio of the peak

Note

This function exposes core peak detection functionality of the *matchedFilter* method. While this function can be called directly, users will generally call the corresponding method for the data object instead (e.g. the `link{findPeaks.matchedFilter}` method).

Author(s)

Colin A Smith, Johannes Rainer

References

Colin A. Smith, Elizabeth J. Want, Grace O'Maille, Ruben Abagyan and Gary Siuzdak. "XCMS: Processing Mass Spectrometry Data for Metabolite Profiling Using Nonlinear Peak Alignment, Matching, and Identification" *Anal. Chem.* 2006, 78:779-787.

See Also

`binYonX` for a binning function, `imputeLinInterpol` for the interpolation of missing values. `matchedFilter` for the standard user interface method.

Other core peak detection functions: `do_findChromPeaks_centWaveWithPredIsoROIs`, `do_findChromPeaks_centWav`
`do_findChromPeaks_massifquant`, `do_findPeaks_MSW`

Examples

```
## Load the test file
library(faahKO)
fs <- system.file('cdf/KO/ko15.CDF', package = "faahKO")
xr <- xcmsRaw(fs)

## Extracting the data from the xcmsRaw for do_findChromPeaks_centWave
mzVals <- xr@env$mz
intVals <- xr@env$intensity
## Define the values per spectrum:
```

```
valsPerSpect <- diff(c(xr@scanindex, length(mzVals)))

res <- do_findChromPeaks_matchedFilter(mz = mzVals, int = intVals,
scantime = xr@scantime, valsPerSpect = valsPerSpect)
head(res)
```

`do_findPeaks_MSW` *Core API function for single-spectrum non-chromatography MS data peak detection*

Description

This function performs peak detection in mass spectrometry direct injection spectrum using a wavelet based algorithm.

Usage

```
do_findPeaks_MSW(mz, int, snthresh = 3, verboseColumns = FALSE, ...)
```

Arguments

`mz`	Numeric vector with the individual m/z values from all scans/ spectra of one file/sample.
`int`	Numeric vector with the individual intensity values from all scans/spectra of one file/sample.
`snthresh`	`numeric(1)` defining the signal to noise ratio cutoff.
`verboseColumns`	`logical(1)` whether additional peak meta data columns should be returned.
`...`	Additional parameters to be passed to the `peakDetectionCWT` function.

Details

This is a wrapper around the peak picker in Bioconductor's `MassSpecWavelet` package calling `peakDetectionCWT` and `tuneInPeakInfo` functions. See the *xcmsDirect* vignette for more information.

Value

A matrix, each row representing an identified peak, with columns:

mz m/z value of the peak at the centroid position.

mzmin Minimum m/z of the peak.

mzmax Maximum m/z of the peak.

rt Always `-1`.

rtmin Always `-1`.

rtmax Always `-1`.

into Integrated (original) intensity of the peak.

maxo Maximum intensity of the peak.

intf Always `NA`.

maxf Maximum MSW-filter response of the peak.

sn Signal to noise ratio.

Author(s)

Joachim Kutzera, Steffen Neumann, Johannes Rainer

See Also

MSW for the standard user interface method. peakDetectionCWT from the MassSpecWavelet package.

Other core peak detection functions: do_findChromPeaks_centWaveWithPredIsoROIs, do_findChromPeaks_centWav
do_findChromPeaks_massifquant, do_findChromPeaks_matchedFilter

---

do_groupChromPeaks_density

Core API function for peak density based chromatographic peak grouping

---

Description

The do_groupChromPeaks_density function performs chromatographic peak grouping based on the density (distribution) of peaks, found in different samples, along the retention time axis in slices of overlapping mz ranges.

Usage

```
do_groupChromPeaks_density(peaks, sampleGroups, bw = 30, minFraction = 0.5,
  minSamples = 1, binSize = 0.25, maxFeatures = 50, sleep = 0)
```

Arguments

peaks	A matrix or data.frame with the mz values and retention times of the identified chromatographic peaks in all samples of an experiment. Required columns are "mz", "rt" and "sample". The latter should contain numeric values representing the index of the sample in which the peak was found.
sampleGroups	A vector of the same length than samples defining the sample group assignments (i.e. which samples belong to which sample group). This parameter is mandatory for the PeakDensityParam and has to be provided also if there is no sample grouping in the experiment (in which case all samples should be assigned to the same group).
bw	numeric(1) defining the bandwidth (standard deviation ot the smoothing kernel) to be used. This argument is passed to the density method.
minFraction	numeric(1) defining the minimum fraction of samples in at least one sample group in which the peaks have to be present to be considered as a peak group (feature).
minSamples	numeric(1) with the minimum number of samples in at least one sample group in which the peaks have to be detected to be considered a peak group (feature).
binSize	numeric(1) defining the size of the overlapping slices in mz dimension.
maxFeatures	numeric(1) with the maximum number of peak groups to be identified in a single mz slice.
sleep	numeric(1) defining the time to *sleep* between iterations and plot the result from the current iteration.

Details

For overlapping slices along the mz dimension, the function calculates the density distribution of identified peaks along the retention time axis and groups peaks from the same or different samples that are close to each other. See [Smith 2006] for more details.

Value

A `list` with elements `"featureDefinitions"` and `"peakIndex"`. `"featureDefinitions"` is a `matrix`, each row representing a (mz-rt) feature (i.e. a peak group) with columns:

"mzmed" median of the peaks' apex mz values.

"mzmin" smallest mz value of all peaks' apex within the feature.

"mzmax" largest mz value of all peaks' apex within the feature.

"rtmed" the median of the peaks' retention times.

"rtmin" the smallest retention time of the peaks in the group.

"rtmax" the largest retention time of the peaks in the group.

"npeaks" the total number of peaks assigned to the feature. Note that this number can be larger than the total number of samples, since multiple peaks from the same sample could be assigned to a feature.

`"peakIndex"` is a `list` with the indices of all peaks in a feature in the `peaks` input matrix.

Note

The default settings might not be appropriate for all LC/GC-MS setups, especially the `bw` and `binSize` parameter should be adjusted accordingly.

Author(s)

Colin Smith, Johannes Rainer

References

Colin A. Smith, Elizabeth J. Want, Grace O'Maille, Ruben Abagyan and Gary Siuzdak. "XCMS: Processing Mass Spectrometry Data for Metabolite Profiling Using Nonlinear Peak Alignment, Matching, and Identification" *Anal. Chem.* 2006, 78:779-787.

See Also

Other core peak grouping algorithms: `do_groupChromPeaks_nearest`, `do_groupPeaks_mzClust`

Examples

```
## Load the test data set
library(faahKO)
data(faahko)

## Extract the matrix with the identified peaks from the xcmsSet:
fts <- peaks(faahko)

## Perform the peak grouping with default settings:
res <- do_groupChromPeaks_density(fts, sampleGroups = sampclass(faahko))
```

```
## The feature definitions:
head(res$featureDefinitions)

## The assignment of peaks from the input matrix to the features
head(res$peakIndex)
```

`do_groupChromPeaks_nearest` *Core API function for chromatic peak grouping using a nearest neighbor approach*

Description

The `do_groupChromPeaks_nearest` function groups peaks across samples by creating a master peak list and assigning corresponding peaks from all samples to each peak group (i.e. feature). The method is inspired by the correspondence algorithm of mzMine [Katajamaa 2006].

Usage

```
do_groupChromPeaks_nearest(peaks, sampleGroups, mzVsRtBalance = 10,
  absMz = 0.2, absRt = 15, kNN = 10)
```

Arguments

`peaks`	A `matrix` or `data.frame` with the mz values and retention times of the identified chromatographic peaks in all samples of an experiment. Required columns are `"mz"`, `"rt"` and `"sample"`. The latter should contain `numeric` values representing the index of the sample in which the peak was found.
`sampleGroups`	A vector of the same length than samples defining the sample group assignments (i.e. which samples belong to which sample group). This parameter is mandatory for the `PeakDensityParam` and has to be provided also if there is no sample grouping in the experiment (in which case all samples should be assigned to the same group).
`mzVsRtBalance`	`numeric(1)` representing the factor by which mz values are multiplied before calculating the (euclician) distance between two peaks.
`absMz`	`numeric(1)` maximum tolerated distance for mz values.
`absRt`	`numeric(1)` maximum tolerated distance for rt values.
`kNN`	`numeric(1)` representing the number of nearest neighbors to check.

Value

A `list` with elements `"featureDefinitions"` and `"peakIndex"`. `"featureDefinitions"` is a `matrix`, each row representing an (mz-rt) feature (i.e. peak group) with columns:

"mzmed" median of the peaks' apex mz values.

"mzmin" smallest mz value of all peaks' apex within the feature.

"mzmax" largest mz value of all peaks' apex within the feature.

"rtmed" the median of the peaks' retention times.

"rtmin" the smallest retention time of the peaks in the feature.

"rtmax" the largest retention time of the peaks in the feature.

"npeaks" the total number of peaks assigned to the feature.

"peakIndex" is a list with the indices of all peaks in a feature in the peaks input matrix.

References

Katajamaa M, Miettinen J, Oresic M: MZmine: Toolbox for processing and visualization of mass spectrometry based molecular profile data. *Bioinformatics* 2006, 22:634-636.

See Also

Other core peak grouping algorithms: do_groupChromPeaks_density, do_groupPeaks_mzClust

---

do_groupPeaks_mzClust *Core API function for peak grouping using mzClust*

Description

The do_groupPeaks_mzClust function performs high resolution correspondence on single spectra samples.

Usage

```
do_groupPeaks_mzClust(peaks, sampleGroups, ppm = 20, absMz = 0,
  minFraction = 0.5, minSamples = 1)
```

Arguments

peaks	A matrix or data.frame with the mz values and retention times of the identified chromatographic peaks in all samples of an experiment. Required columns are "mz", "rt" and "sample". The latter should contain numeric values representing the index of the sample in which the peak was found.
sampleGroups	A vector of the same length than samples defining the sample group assignments (i.e. which samples belong to which sample group). This parameter is mandatory for the PeakDensityParam and has to be provided also if there is no sample grouping in the experiment (in which case all samples should be assigned to the same group).
ppm	numeric(1) representing the relative mz error for the clustering/grouping (in parts per million).
absMz	numeric(1) representing the absolute mz error for the clustering.
minFraction	numeric(1) defining the minimum fraction of samples in at least one sample group in which the peaks have to be present to be considered as a peak group (feature).
minSamples	numeric(1) with the minimum number of samples in at least one sample group in which the peaks have to be detected to be considered a peak group (feature).

Value

A `list` with elements `"featureDefinitions"` and `"peakIndex"`. `"featureDefinitions"` is a `matrix`, each row representing an (mz-rt) feature (i.e. peak group) with columns:

"mzmed" median of the peaks' apex mz values.

"mzmin" smallest mz value of all peaks' apex within the feature.

"mzmax" largest mz value of all peaks' apex within the feature.

"rtmed" always `-1`.

"rtmin" always `-1`.

"rtmax" always `-1`.

"npeaks" the total number of peaks assigned to the feature. Note that this number can be larger than the total number of samples, since multiple peaks from the same sample could be assigned to a group.

`"peakIndex"` is a `list` with the indices of all peaks in a peak group in the `peaks` input matrix.

References

Saira A. Kazmi, Samiran Ghosh, Dong-Guk Shin, Dennis W. Hill and David F. Grant
Alignment of high resolution mass spectra: development of a heuristic approach for metabolomics.
Metabolomics, Vol. 2, No. 2, 75-83 (2006)

See Also

Other core peak grouping algorithms: `do_groupChromPeaks_density`, `do_groupChromPeaks_nearest`

`etg` *Empirically Transformed Gaussian function*

Description

A general function for asymmetric chromatographic peaks.

Usage

```
etg(x, H, t1, tt, k1, kt, lambda1, lambdat, alpha, beta)
```

Arguments

`x`	times to evaluate function at
`H`	peak height
`t1`	time of leading edge inflection point
`tt`	time of trailing edge inflection point
`k1`	leading edge parameter
`kt`	trailing edge parameter
`lambda1`	leading edge parameter
`lambdat`	trailing edge parameter
`alpha`	leading edge parameter
`beta`	trailing edge parameter

Value

The function evaluated at times x.

Author(s)

Colin A. Smith, <csmith@scripps.edu>

References

Jianwei Li. Development and Evaluation of Flexible Empirical Peak Functions for Processing Chromatographic Peaks. Anal. Chem., 69 (21), 4452-4462, 1997. http://dx.doi.org/10.1021/ac970481d

---

`extractMsData,OnDiskMSnExp-method`

Extract a `data.frame` *containing MS data*

Description

Extract a `data.frame` of retention time, mz and intensity values from each file/sample in the provided rt-mz range (or for the full data range if `rt` and `mz` are not defined).

Usage

```
## S4 method for signature 'OnDiskMSnExp'
extractMsData(object, rt, mz, msLevel = 1L)

## S4 method for signature 'XCMSnExp'
extractMsData(object, rt, mz, msLevel = 1L,
  adjustedRtime = hasAdjustedRtime(object))
```

Arguments

`object`	A `XCMSnExp` or `OnDiskMSnExp` object.
`rt`	`numeric(2)` with the retention time range from which the data should be extracted.
`mz`	`numeric(2)` with the mz range.
`msLevel`	`integer` defining the MS level(s) to which the data should be sub-setted prior to extraction; defaults to `msLevel = 1L`.
`adjustedRtime`	(for `extractMsData,XCMSnExp`): `logical(1)` specifying if adjusted or raw retention times should be reported. Defaults to adjusted retention times, if these are present in `object`.

Value

A `list` of length equal to the number of samples/files in `object`. Each element being a `data.frame` with columns `"rt"`, `"mz"` and `"i"` with the retention time, mz and intensity tuples of a file. If no data is available for the mz-rt range in a file a `data.frame` with 0 rows is returned for that file.

Author(s)

Johannes Rainer

See Also

XCMSnExp for the data object. plotMsData to plot the data for a single file.

Examples

```
## Read some files from the test data package.
library(faahKO)
library(xcms)
fls <- dir(system.file("cdf/KO", package = "faahKO"), recursive = TRUE,
           full.names = TRUE)
raw_data <- readMSData(fls[1:2], mode = "onDisk")

## Read the full MS data for a defined mz-rt region.
res <- extractMsData(raw_data, mz = c(300, 320), rt = c(2700, 2900))

## We've got one data.frame per file
length(res)

## With number of rows:
nrow(res[[1]])

head(res[[1]])
```

---

featureValues,XCMSnExp-method

Accessing mz-rt feature data values

Description

featureValues,XCMSnExp : extract a matrix for feature values with rows representing features and columns samples. Parameter value allows to define which column from the chromPeaks matrix should be returned. Multiple chromatographic peaks from the same sample can be assigned to a feature. Parameter method allows to specify the method to be used in such cases to chose from which of the peaks the value should be returned.

Usage

```
## S4 method for signature 'XCMSnExp'
featureValues(object, method = c("medret", "maxint"),
  value = "index", intensity = "into", filled = TRUE)
```

Arguments

object	A XCMSnExp object providing the feature definitions.
method	character specifying the method to resolve multi-peak mappings within the same sample, i.e. to define the *representative* peak for a feature in samples where more than one peak was assigned to the feature. If "medret": select the peak closest to the median retention time of the feature. If "maxint": select the peak yielding the largest signal.

value — character specifying the name of the column in chromPeaks(object) that should be returned or "index" (the default) to return the index of the peak in the chromPeaks(object) matrix corresponding to the *representative* peak for the feature in the respective sample.

intensity — character specifying the name of the column in the chromPeaks(objects) matrix containing the intensity value of the peak that should be used for the conflict resolution if method = "maxint".

filled — logical(1) specifying whether values for filled-in peaks should be returned or not. If filled = FALSE, an NA is returned in the matrix for the respective peak. See fillChromPeaks for details on peak filling.

Value

For featureValues: a matrix with feature values, columns representing samples, rows features. The order of the features matches the order found in the featureDefinitions(object) DataFrame. The rownames of the matrix are the same than those of the featureDefinitions DataFrame. NA is reported for features without corresponding chromatographic peak in the respective sample(s).

Note

This method is equivalent to the groupval for xcmsSet objects.

Author(s)

Johannes Rainer

See Also

XCMSnExp for information on the data object. featureDefinitions to extract the DataFrame with the feature definitions. hasFeatures to evaluate whether the XCMSnExp provides feature definitions. groupval for the equivalent method on xcmsSet objects.

FillChromPeaksParam-class

Integrate areas of missing peaks

Description

The FillChromPeaksParam object encapsules all settings for the signal integration for missing peaks.

expandMz,expandMz<-: getter and setter for the expandMz slot of the object.

expandRt,expandRt<-: getter and setter for the expandRt slot of the object.

ppm,ppm<-: getter and setter for the ppm slot of the object.

Integrate signal in the mz-rt area of a feature (chromatographic peak group) for samples in which no chromatographic peak for this feature was identified and add it to the chromPeaks. Such peaks will have a value of 1 in the "is_filled" column of the chromPeaks matrix of the object.

Usage

```
FillChromPeaksParam(expandMz = 0, expandRt = 0, ppm = 0)

## S4 method for signature 'FillChromPeaksParam'
show(object)

## S4 method for signature 'FillChromPeaksParam'
expandMz(object)

## S4 replacement method for signature 'FillChromPeaksParam'
expandMz(object) <- value

## S4 method for signature 'FillChromPeaksParam'
expandRt(object)

## S4 replacement method for signature 'FillChromPeaksParam'
expandRt(object) <- value

## S4 method for signature 'FillChromPeaksParam'
ppm(object)

## S4 replacement method for signature 'FillChromPeaksParam'
ppm(object) <- value

## S4 method for signature 'XCMSnExp,FillChromPeaksParam'
fillChromPeaks(object, param,
  BPPARAM = bpparam())

## S4 method for signature 'XCMSnExp,missing'
fillChromPeaks(object, param,
  BPPARAM = bpparam())
```

Arguments

expandMz	numeric(1) defining the value by which the mz width of peaks should be expanded. Each peak is expanded in mz direction by expandMz * their original mz width. A value of 0 means no expansion, a value of 1 grows each peak by 1 * the mz width of the peak resulting in peakswith twice their original size in mz direction (expansion by half mz width to both sides).
expandRt	numeric(1), same as expandRt but for the retention time width.
ppm	numeric(1) optionally specifying a *ppm* by which the mz width of the peak region should be expanded. For peaks with an mz width smaller than mean(c(mzmin, mzmax)) * ppm / the mzmin will be replaced by mean(c(mzmin, mzmax)) - (mean(c(mzmin, mzmax)) * ppm / 2 / and mzmax by mean(c(mzmin, mzmax)) + (mean(c(mzmin, mzmax)) * ppm / 2 / 1e6). This is applied before eventually expanding the mz width using the expandMz parameter.
object	XCMSnExp object with identified and grouped chromatographic peaks.
value	The value for the slot.
param	A FillChromPeaksParam object with all settings.
BPPARAM	Parallel processing settings.

Details

After correspondence (i.e. grouping of chromatographic peaks across samples) there will always be features (peak groups) that do not include peaks from every sample. The `fillChromPeaks` method defines intensity values for such features in the missing samples by integrating the signal in the mz-rt region of the feature. The mz-rt area is defined by the median mz and rt start and end points of the other detected chromatographic peaks for a given feature.

Adjusted retention times will be used if available.

Based on the peak finding algorithm that was used to identify the (chromatographic) peaks different internal functions are employed to guarantee that the integrated peak signal matches as much as possible the peak signal integration used during the peak detection. For peaks identified with the `matchedFilter` method, signal integration is performed on the *profile matrix* generated with the same settings used also during peak finding (using the same `bin` size for example). For direct injection data and peaks identified with the `MSW` algorithm signal is integrated only along the mz dimension. For all other methods the complete (raw) signal within the area defined by `"mzmin"`, `"mzmax"`, `"rtmin"` and `"rtmax"` is used.

Value

The `FillChromPeaksParam` function returns a `FillChromPeaksParam` object.

A `XCMSnExp` object with previously missing chromatographic peaks for features filled into its `chromPeaks` matrix.

Slots

`.__classVersion__,expandMz,expandRt,ppm` See corresponding parameter above. `.__classVersion__` stores the version of the class.

Note

The reported `"mzmin"`, `"mzmax"`, `"rtmin"` and `"rtmax"` for the filled peaks represents the actual MS area from which the signal was integrated. Note that no peak is filled in if no signal was present in a file/sample in the respective mz-rt area. These samples will still show a `NA` in the matrix returned by the `featureValues` method. This is in contrast to the `fillPeaks.chrom` method that returned an `"into"` and `"maxo"` of `0` for such peak areas. Growing the mz-rt area using the `expandMz` and `expandRt` might help to reduce the number of missing peak signals after filling.

Author(s)

Johannes Rainer

See Also

`groupChromPeaks` for methods to perform the correspondence. `dropFilledChromPeaks` for the method to remove filled in peaks.

Examples

```
## Perform the peak detection using centWave on some of the files from the
## faahKO package. Files are read using the readMSData from the MSnbase
## package
library(faahKO)
library(xcms)
```

```
fls <- dir(system.file("cdf/KO", package = "faahKO"), recursive = TRUE,
           full.names = TRUE)
raw_data <- readMSData(fls[1:2], mode = "onDisk")

## Create a CentWaveParam object. Note that the noise is set to 10000 to
## speed up the execution of the example - in a real use case the default
## value should be used, or it should be set to a reasonable value.
cwp <- CentWaveParam(ppm = 20, noise = 10000, snthresh = 40)

res <- findChromPeaks(raw_data, param = cwp)

## Perform the correspondence. We assign all samples to the same group.
res <- groupChromPeaks(res,
    param = PeakDensityParam(sampleGroups = rep(1, length(fileNames(res)))))

## For how many features do we lack an integrated peak signal?
sum(is.na(featureValues(res)))

## Filling missing peak data using default settings.
res <- fillChromPeaks(res)

## Get the peaks that have been filled in:
fp <- chromPeaks(res)[chromPeaks(res)[, "is_filled"] == 1, ]
head(fp)

## Did we get a signal for all missing peaks?
sum(is.na(featureValues(res)))

## No.

## Get the process history step along with the parameters used to perform
## The peak filling:
ph <- processHistory(res, type = "Missing peak filling")[[1]]
ph

## The parameter class:
ph@param

## Drop the filled in peaks:
res <- dropFilledChromPeaks(res)

## Perform the peak filling with modified settings: allow expansion of the
## mz range by a specified ppm and expanding the mz range by mz width/2
prm <- FillChromPeaksParam(ppm = 40, expandMz = 0.5)
res <- fillChromPeaks(res, param = prm)

## Did we get a signal for all missing peaks?
sum(is.na(featureValues(res)))

## Still the same missing peaks.
```

`fillPeaks-methods` *Integrate areas of missing peaks*

Description

For each sample, identify peak groups where that sample is not represented. For each of those peak groups, integrate the signal in the region of that peak group and create a new peak.

Arguments

object	the xcmsSet object
method	the filling method

Details

After peak grouping, there will always be peak groups that do not include peaks from every sample. This method produces intensity values for those missing samples by integrating raw data in peak group region. According to the type of raw-data there are 2 different methods available. for filling gcms/lcms data the method "chrom" integrates raw-data in the chromatographic domain, whereas "MSW" is used for peaklists without retention-time information like those from direct-infusion spectra.

Value

A xcmsSet objects with filled in peak groups.

Methods

object = "xcmsSet" `fillPeaks(object, method="")`

See Also

xcmsSet-class, getPeaks

---

fillPeaks.chrom-methods

Integrate areas of missing peaks

Description

For each sample, identify peak groups where that sample is not represented. For each of those peak groups, integrate the signal in the region of that peak group and create a new peak.

Arguments

object	the xcmsSet object
nSlaves	(DEPRECATED): number of slaves/cores to be used for parallel peak filling. MPI is used if installed, otherwise the snow package is employed for multicore support. If none of the two packages is available it uses the parallel package for parallel processing on multiple CPUs of the current machine. Users are advised to use the BPPARAM parameter instead.
expand.mz	Expansion factor for the m/z range used for integration.
expand.rt	Expansion factor for the rentention time range used for integration.
BPPARAM	allows to define a specific parallel processing setup for the current task (see bpparam from the BiocParallel package help more information). The default uses the globally defined parallel setup.

Details

After peak grouping, there will always be peak groups that do not include peaks from every sample. This method produces intensity values for those missing samples by integrating raw data in peak group region. In a given group, the start and ending retention time points for integration are defined by the median start and end points of the other detected peaks. The start and end m/z values are similarly determined. Intensities can be still be zero, which is a rather unusual intensity for a peak. This is the case if e.g. the raw data was threshholded, and the integration area contains no actual raw intensities, or if one sample is miscalibrated, such thet the raw data points are (just) outside the integration area.

Importantly, if retention time correction data is available, the alignment information is used to more precisely integrate the propper region of the raw data. If the corrected retention time is beyond the end of the raw data, the value will be not-a-number (NaN).

Value

A `xcmsSet` objects with filled in peak groups (into and maxo).

Methods

object = "xcmsSet" `fillPeaks.chrom(object, nSlaves=0,expand.mz=1,expand.rt=1,  BPPARAM = bpparam(`

See Also

`xcmsSet-class`, `getPeaks` `fillPeaks`

`fillPeaks.MSW-methods` *Integrate areas of missing peaks in FTICR-MS data*

Description

For each sample, identify peak groups where that sample is not represented. For each of those peak groups, integrate the signal in the region of that peak group and create a new peak.

Arguments

`object`	the `xcmsSet` object

Details

After peak grouping, there will always be peak groups that do not include peaks from every sample. This method produces intensity values for those missing samples by integrating raw data in peak group region. In a given group, the start and ending m/z values for integration are defined by the median start and end points of the other detected peaks.

Value

A `xcmsSet` objects with filled in peak groups.

Methods

object = "xcmsSet" `fillPeaks.MSW(object)`

Note

In contrast to the fillPeaks.chrom method the maximum intensity reported in column "maxo" is not the maximum intensity measured in the expected peak area (defined by columns "mzmin" and "mzmax"), but the largest intensity of mz value(s) closest to the "mzmed" of the feature.

See Also

xcmsSet-class, getPeaks fillPeaks

---

findChromPeaks-centWave

Chromatographic peak detection using the centWave method

Description

The centWave algorithm perform peak density and wavelet based chromatographic peak detection for high resolution LC/MS data in centroid mode [Tautenhahn 2008].

The CentWaveParam class allows to specify all settings for a chromatographic peak detection using the centWave method. Instances should be created with the CentWaveParam constructor.

The detectChromPeaks,OnDiskMSnExp,CentWaveParam method performs chromatographic peak detection using the *centWave* algorithm on all samples from an OnDiskMSnExp object. OnDiskMSnExp objects encapsule all experiment specific data and load the spectra data (mz and intensity values) on the fly from the original files applying also all eventual data manipulations.

ppm,ppm<-: getter and setter for the ppm slot of the object.

peakwidth,peakwidth<-: getter and setter for the peakwidth slot of the object.

snthresh,snthresh<-: getter and setter for the snthresh slot of the object.

prefilter,prefilter<-: getter and setter for the prefilter slot of the object.

mzCenterFun,mzCenterFun<-: getter and setter for the mzCenterFun slot of the object.

integrate,integrate<-: getter and setter for the integrate slot of the object.

mzdiff,mzdiff<-: getter and setter for the mzdiff slot of the object.

fitgauss,fitgauss<-: getter and setter for the fitgauss slot of the object.

noise,noise<-: getter and setter for the noise slot of the object.

verboseColumns,verboseColumns<-: getter and setter for the verboseColumns slot of the object.

roiList,roiList<-: getter and setter for the roiList slot of the object.

fistBaselineCheck,firstBaselineCheck<-: getter and setter for the firstBaselineCheck slot of the object.

roiScales,roiScales<-: getter and setter for the roiScales slot of the object.

Usage

```
CentWaveParam(ppm = 25, peakwidth = c(20, 50), snthresh = 10,
  prefilter = c(3, 100), mzCenterFun = "wMean", integrate = 1L,
  mzdiff = -0.001, fitgauss = FALSE, noise = 0, verboseColumns = FALSE,
  roiList = list(), firstBaselineCheck = TRUE, roiScales = numeric())

## S4 method for signature 'OnDiskMSnExp,CentWaveParam'
```

```
findChromPeaks(object, param,
  BPPARAM = bpparam(), return.type = "XCMSnExp", msLevel = 1L)

## S4 method for signature 'CentWaveParam'
show(object)

## S4 method for signature 'CentWaveParam'
ppm(object)

## S4 replacement method for signature 'CentWaveParam'
ppm(object) <- value

## S4 method for signature 'CentWaveParam'
peakwidth(object)

## S4 replacement method for signature 'CentWaveParam'
peakwidth(object) <- value

## S4 method for signature 'CentWaveParam'
snthresh(object)

## S4 replacement method for signature 'CentWaveParam'
snthresh(object) <- value

## S4 method for signature 'CentWaveParam'
prefilter(object)

## S4 replacement method for signature 'CentWaveParam'
prefilter(object) <- value

## S4 method for signature 'CentWaveParam'
mzCenterFun(object)

## S4 replacement method for signature 'CentWaveParam'
mzCenterFun(object) <- value

## S4 method for signature 'CentWaveParam'
integrate(f)

## S4 replacement method for signature 'CentWaveParam'
integrate(object) <- value

## S4 method for signature 'CentWaveParam'
mzdiff(object)

## S4 replacement method for signature 'CentWaveParam'
mzdiff(object) <- value

## S4 method for signature 'CentWaveParam'
fitgauss(object)

## S4 replacement method for signature 'CentWaveParam'
```

```
fitgauss(object) <- value

## S4 method for signature 'CentWaveParam'
noise(object)

## S4 replacement method for signature 'CentWaveParam'
noise(object) <- value

## S4 method for signature 'CentWaveParam'
verboseColumns(object)

## S4 replacement method for signature 'CentWaveParam'
verboseColumns(object) <- value

## S4 method for signature 'CentWaveParam'
roiList(object)

## S4 replacement method for signature 'CentWaveParam'
roiList(object) <- value

## S4 method for signature 'CentWaveParam'
firstBaselineCheck(object)

## S4 replacement method for signature 'CentWaveParam'
firstBaselineCheck(object) <- value

## S4 method for signature 'CentWaveParam'
roiScales(object)

## S4 replacement method for signature 'CentWaveParam'
roiScales(object) <- value
```

Arguments

ppm	numeric(1) defining the maximal tolerated m/z deviation in consecutive scans in parts per million (ppm) for the initial ROI definition.
peakwidth	numeric(2) with the expected approximate peak width in chromatographic space. Given as a range (min, max) in seconds.
snthresh	numeric(1) defining the signal to noise ratio cutoff.
prefilter	numeric(2): c(k, I) specifying the prefilter step for the first analysis step (ROI detection). Mass traces are only retained if they contain at least k peaks with intensity >= I.
mzCenterFun	Name of the function to calculate the m/z center of the chromatographic peak. Allowed are: "wMean": intensity weighted mean of the peak's m/z values, "mean": mean of the peak's m/z values, "apex": use the m/z value at the peak apex, "wMeanApex3": intensity weighted mean of the m/z value at the peak apex and the m/z values left and right of it and "meanApex3": mean of the m/z value of the peak apex and the m/z values left and right of it.
integrate	Integration method. For integrate = 1 peak limits are found through descent on the mexican hat filtered data, for integrate = 2 the descent is done on the real data. The latter method is more accurate but prone to noise, while the former is more robust, but less exact.

mzdiff	numeric(1) representing the minimum difference in m/z dimension for peaks with overlapping retention times; can be negatove to allow overlap.
fitgauss	logical(1) whether or not a Gaussian should be fitted to each peak.
noise	numeric(1) allowing to set a minimum intensity required for centroids to be considered in the first analysis step (centroids with intensity < noise are omitted from ROI detection).
verboseColumns	logical(1) whether additional peak meta data columns should be returned.
roiList	An optional list of regions-of-interest (ROI) representing detected mass traces. If ROIs are submitted the first analysis step is omitted and chromatographic peak detection is performed on the submitted ROIs. Each ROI is expected to have the following elements specified: scmin (start scan index), scmax (end scan index), mzmin (minimum m/z), mzmax (maximum m/z), length (number of scans), intensity (summed intensity). Each ROI should be represented by a list of elements or a single row data.frame.
firstBaselineCheck	logical(1). If TRUE continuous data within regions of interest is checked to be above the first baseline.
roiScales	Optional numeric vector with length equal to roiList defining the scale for each region of interest in roiList that should be used for the centWave-wavelets.
object	For findChromPeaks: an OnDiskMSnExp object containing the MS- and all other experiment-relevant data. For all other methods: a parameter object.
param	An CentWaveParam object containing all settings for the centWave algorithm.
BPPARAM	A parameter class specifying if and how parallel processing should be performed. It defaults to bpparam. See documentation of the BiocParallel for more details. If parallel processing is enabled, peak detection is performed in parallel on several of the input samples.
return.type	Character specifying what type of object the method should return. Can be either "XCMSnExp" (default), "list" or "xcmsSet".
msLevel	integer(1) defining the MS level on which the peak detection should be performed. Defaults to msLevel = 1.
value	The value for the slot.
f	For integrate: a CentWaveParam object.

Details

The centWave algorithm is most suitable for high resolution LC/{TOF,OrbiTrap,FTICR}-MS data in centroid mode. In the first phase the method identifies *regions of interest* (ROIs) representing mass traces that are characterized as regions with less than ppm m/z deviation in consecutive scans in the LC/MS map. These ROIs are then subsequently analyzed using continuous wavelet transform (CWT) to locate chromatographic peaks on different scales. The first analysis step is skipped, if regions of interest are passed *via* the param parameter.

Parallel processing (one process per sample) is supported and can be configured either by the BPPARAM parameter or by globally defining the parallel processing mode using the register method from the BiocParallel package.

Value

The CentWaveParam function returns a CentWaveParam class instance with all of the settings specified for chromatographic peak detection by the centWave method.

For findChromPeaks: if return.type = "XCMSnExp" an XCMSnExp object with the results of the peak detection. If return.type = "list" a list of length equal to the number of samples with matrices specifying the identified peaks. If return.type = "xcmsSet" an xcmsSet object with the results of the peak detection.

Slots

.__classVersion__,ppm,peakwidth,snthresh,prefilter,mzCenterFun,integrate,mzdiff,fitgauss,noise,v
: See corresponding parameter above. .__classVersion__ stores the version from the class. Slots values should exclusively be accessed *via* the corresponding getter and setter methods listed above.

Note

These methods and classes are part of the updated and modernized xcms user interface which will eventually replace the findPeaks methods. It supports peak detection on MSnExp and OnDiskMSnExp objects (both defined in the MSnbase package). All of the settings to the centWave algorithm can be passed with a CentWaveParam object.

Author(s)

Ralf Tautenhahn, Johannes Rainer

References

Ralf Tautenhahn, Christoph B\"ottcher, and Steffen Neumann "Highly sensitive feature detection for high resolution LC/MS" *BMC Bioinformatics* 2008, 9:504

See Also

The do_findChromPeaks_centWave core API function and findPeaks.centWave for the old user interface.

XCMSnExp for the object containing the results of the peak detection.

Other peak detection methods: chromatographic-peak-detection, findChromPeaks-centWaveWithPredIsoROIs, findChromPeaks-massifquant, findChromPeaks-matchedFilter, findPeaks-MSW

Examples

```
## Create a CentWaveParam object. Note that the noise is set to 10000 to
## speed up the execution of the example - in a real use case the default
## value should be used, or it should be set to a reasonable value.
cwp <- CentWaveParam(ppm = 20, noise = 10000)
## Change snthresh parameter
snthresh(cwp) <- 25
cwp

## Perform the peak detection using centWave on some of the files from the
## faahKO package. Files are read using the readMSData from the MSnbase
## package
```

```
library(faahKO)
library(xcms)
fls <- dir(system.file("cdf/KO", package = "faahKO"), recursive = TRUE,
           full.names = TRUE)
raw_data <- readMSData(fls[1:2], mode = "onDisk")

## Perform the peak detection using the settings defined above.
res <- findChromPeaks(raw_data, param = cwp)
head(chromPeaks(res))
```

`findChromPeaks-centWaveWithPredIsoROIs` *Two-step centWave peak detection considering also isotopes*

Description

This method performs a two-step centWave-based chromatographic peak detection: in a first centWave run peaks are identified for which then the location of their potential isotopes in the mz-retention time is predicted. A second centWave run is then performed on these *regions of interest* (ROIs). The final list of chromatographic peaks comprises all non-overlapping peaks from both centWave runs.

The `CentWavePredIsoParam` class allows to specify all settings for the two-step centWave-based peak detection considering also predicted isotopes of peaks identified in the first centWave run. Instances should be created with the `CentWavePredIsoParam` constructor. See also the documentation of the `CentWaveParam` for all methods and arguments this class inherits.

The `findChromPeaks,OnDiskMSnExp,CentWavePredIsoParam` method performs a two-step centWave-based chromatographic peak detection on all samples from an `OnDiskMSnExp` object. `OnDiskMSnExp` objects encapsule all experiment specific data and load the spectra data (mz and intensity values) on the fly from the original files applying also all eventual data manipulations.

`snthreshIsoROIs,snthreshIsoROIs<-`: getter and setter for the `snthreshIsoROIs` slot of the object.

`maxCharge,maxCharge<-`: getter and setter for the `maxCharge` slot of the object.

`maxIso,maxIso<-`: getter and setter for the `maxIso` slot of the object.

`mzIntervalExtension,mzIntervalExtension<-`: getter and setter for the `mzIntervalExtension` slot of the object.

`polarity,polarity<-`: getter and setter for the `polarity` slot of the object.

Usage

```
CentWavePredIsoParam(ppm = 25, peakwidth = c(20, 50), snthresh = 10,
  prefilter = c(3, 100), mzCenterFun = "wMean", integrate = 1L,
  mzdiff = -0.001, fitgauss = FALSE, noise = 0, verboseColumns = FALSE,
  roiList = list(), firstBaselineCheck = TRUE, roiScales = numeric(),
  snthreshIsoROIs = 6.25, maxCharge = 3, maxIso = 5,
  mzIntervalExtension = TRUE, polarity = "unknown")

## S4 method for signature 'OnDiskMSnExp,CentWavePredIsoParam'
findChromPeaks(object, param,
  BPPARAM = bpparam(), return.type = "XCMSnExp", msLevel = 1L)
```

```
## S4 method for signature 'CentWavePredIsoParam'
show(object)

## S4 method for signature 'CentWavePredIsoParam'
snthreshIsoROIs(object)

## S4 replacement method for signature 'CentWavePredIsoParam'
snthreshIsoROIs(object) <- value

## S4 method for signature 'CentWavePredIsoParam'
maxCharge(object)

## S4 replacement method for signature 'CentWavePredIsoParam'
maxCharge(object) <- value

## S4 method for signature 'CentWavePredIsoParam'
maxIso(object)

## S4 replacement method for signature 'CentWavePredIsoParam'
maxIso(object) <- value

## S4 method for signature 'CentWavePredIsoParam'
mzIntervalExtension(object)

## S4 replacement method for signature 'CentWavePredIsoParam'
mzIntervalExtension(object) <- value

## S4 method for signature 'CentWavePredIsoParam'
polarity(object)

## S4 replacement method for signature 'CentWavePredIsoParam'
polarity(object) <- value
```

Arguments

ppm	numeric(1) defining the maximal tolerated m/z deviation in consecutive scans in parts per million (ppm) for the initial ROI definition.
peakwidth	numeric(2) with the expected approximate peak width in chromatographic space. Given as a range (min, max) in seconds.
snthresh	numeric(1) defining the signal to noise ratio cutoff.
prefilter	numeric(2): c(k, I) specifying the prefilter step for the first analysis step (ROI detection). Mass traces are only retained if they contain at least k peaks with intensity >= I.
mzCenterFun	Name of the function to calculate the m/z center of the chromatographic peak. Allowed are: "wMean": intensity weighted mean of the peak's m/z values, "mean": mean of the peak's m/z values, "apex": use the m/z value at the peak apex, "wMeanApex3": intensity weighted mean of the m/z value at the peak apex and the m/z values left and right of it and "meanApex3": mean of the m/z value of the peak apex and the m/z values left and right of it.
integrate	Integration method. For integrate = 1 peak limits are found through descent on the mexican hat filtered data, for integrate = 2 the descent is done on

the real data. The latter method is more accurate but prone to noise, while the former is more robust, but less exact.

`mzdiff` `numeric(1)` representing the minimum difference in m/z dimension for peaks with overlapping retention times; can be negatove to allow overlap.

`fitgauss` `logical(1)` whether or not a Gaussian should be fitted to each peak.

`noise` `numeric(1)` allowing to set a minimum intensity required for centroids to be considered in the first analysis step (centroids with intensity < `noise` are omitted from ROI detection).

`verboseColumns` `logical(1)` whether additional peak meta data columns should be returned.

`roiList` An optional list of regions-of-interest (ROI) representing detected mass traces. If ROIs are submitted the first analysis step is omitted and chromatographic peak detection is performed on the submitted ROIs. Each ROI is expected to have the following elements specified: `scmin` (start scan index), `scmax` (end scan index), `mzmin` (minimum m/z), `mzmax` (maximum m/z), `length` (number of scans), `intensity` (summed intensity). Each ROI should be represented by a `list` of elements or a single row `data.frame`.

`firstBaselineCheck`
`logical(1)`. If `TRUE` continuous data within regions of interest is checked to be above the first baseline.

`roiScales` Optional numeric vector with length equal to `roiList` defining the scale for each region of interest in `roiList` that should be used for the centWave-wavelets.

`snthreshIsoROIs`
`numeric(1)` defining the signal to noise ratio cutoff to be used in the second centWave run to identify peaks for predicted isotope ROIs.

`maxCharge` `integer(1)` defining the maximal isotope charge. Isotopes will be defined for charges `1:maxCharge`.

`maxIso` `integer(1)` defining the number of isotope peaks that should be predicted for each peak identified in the first centWave run.

`mzIntervalExtension`
`logical(1)` whether the mz range for the predicted isotope ROIs should be extended to increase detection of low intensity peaks.

`polarity` `character(1)` specifying the polarity of the data. Currently not used, but has to be `"positive"`, `"negative"` or `"unknown"` if provided.

`object` For `findChromPeaks`: an `OnDiskMSnExp` object containing the MS- and all other experiment-relevant data.
For all other methods: a parameter object.

`param` An `CentWavePredIsoParam` object with the settings for the chromatographic peak detection algorithm.

`BPPARAM` A parameter class specifying if and how parallel processing should be performed. It defaults to `bpparam`. See documentation of the `BiocParallel` for more details. If parallel processing is enabled, peak detection is performed in parallel on several of the input samples.

`return.type` Character specifying what type of object the method should return. Can be either `"XCMSnExp"` (default), `"list"` or `"xcmsSet"`.

`msLevel` `integer(1)` defining the MS level on which the peak detection should be performed. Defaults to `msLevel = 1`.

`value` The value for the slot.

Details

See centWave for details on the centWave method.

Parallel processing (one process per sample) is supported and can be configured either by the BPPARAM parameter or by globally defining the parallel processing mode using the register method from the BiocParallel package.

Value

The CentWavePredIsoParam function returns a CentWavePredIsoParam class instance with all of the settings specified for the two-step centWave-based peak detection considering also isotopes.

For findChromPeaks: if return.type = "XCMSnExp" an XCMSnExp object with the results of the peak detection. If return.type = "list" a list of length equal to the number of samples with matrices specifying the identified peaks. If return.type = "xcmsSet" an xcmsSet object with the results of the peak detection.

Slots

.__classVersion__,ppm,peakwidth,snthresh,prefilter,mzCenterFun,integrate,mzdiff,fitgauss,noise,v
: See corresponding parameter above. .__classVersion__ stores the version from the class. Slots values should exclusively be accessed *via* the corresponding getter and setter methods listed above.

Note

These methods and classes are part of the updated and modernized xcms user interface which will eventually replace the findPeaks methods. It supports chromatographic peak detection on MSnExp and OnDiskMSnExp objects (both defined in the MSnbase package). All of the settings to the algorithm can be passed with a CentWavePredIsoParam object.

Author(s)

Hendrik Treutler, Johannes Rainer

See Also

The do_findChromPeaks_centWaveWithPredIsoROIs core API function and findPeaks.centWave for the old user interface. CentWaveParam for the class the CentWavePredIsoParam extends.

XCMSnExp for the object containing the results of the peak detection.

Other peak detection methods: chromatographic-peak-detection, findChromPeaks-centWave, findChromPeaks-massifquant, findChromPeaks-matchedFilter, findPeaks-MSW

Examples

```
## Create a param object
p <- CentWavePredIsoParam(maxCharge = 4)
## Change snthresh parameter
snthresh(p) <- 25
p
```

findChromPeaks-massifquant

Chromatographic peak detection using the massifquant method

Description

Massifquant is a Kalman filter (KF)-based chromatographic peak detection for XC-MS data in centroid mode. The identified peaks can be further refined with the *centWave* method (see findChromPeaks-centWave for details on centWave) by specifying withWave = TRUE.

The MassifquantParam class allows to specify all settings for a chromatographic peak detection using the massifquant method eventually in combination with the centWave algorithm. Instances should be created with the MassifquantParam constructor.

The findChromPeaks,OnDiskMSnExp,MassifquantParam method performs chromatographic peak detection using the *massifquant* algorithm on all samples from an OnDiskMSnExp object. OnDiskMSnExp objects encapsule all experiment specific data and load the spectra data (mz and intensity values) on the fly from the original files applying also all eventual data manipulations.

ppm,ppm<-: getter and setter for the ppm slot of the object.

peakwidth,peakwidth<-: getter and setter for the peakwidth slot of the object.

snthresh,snthresh<-: getter and setter for the snthresh slot of the object.

prefilter,prefilter<-: getter and setter for the prefilter slot of the object.

mzCenterFun,mzCenterFun<-: getter and setter for the mzCenterFun slot of the object.

integrate,integrate<-: getter and setter for the integrate slot of the object.

mzdiff,mzdiff<-: getter and setter for the mzdiff slot of the object.

fitgauss,fitgauss<-: getter and setter for the fitgauss slot of the object.

noise,noise<-: getter and setter for the noise slot of the object.

verboseColumns,verboseColumns<-: getter and setter for the verboseColumns slot of the object.

criticalValue,criticalValue<-: getter and setter for the criticalValue slot of the object.

consecMissedLimit,consecMissedLimit<-: getter and setter for the consecMissedLimit slot of the object.

unions,unions<-: getter and setter for the unions slot of the object.

checkBack,checkBack<-: getter and setter for the checkBack slot of the object.

withWave,withWave<-: getter and setter for the withWave slot of the object.

Usage

```
MassifquantParam(ppm = 25, peakwidth = c(20, 50), snthresh = 10,
  prefilter = c(3, 100), mzCenterFun = "wMean", integrate = 1L,
  mzdiff = -0.001, fitgauss = FALSE, noise = 0, verboseColumns = FALSE,
  criticalValue = 1.125, consecMissedLimit = 2, unions = 1,
  checkBack = 0, withWave = FALSE)

## S4 method for signature 'OnDiskMSnExp,MassifquantParam'
findChromPeaks(object, param,
  BPPARAM = bpparam(), return.type = "XCMSnExp", msLevel = 1L)
```

```
## S4 method for signature 'MassifquantParam'
show(object)

## S4 method for signature 'MassifquantParam'
ppm(object)

## S4 replacement method for signature 'MassifquantParam'
ppm(object) <- value

## S4 method for signature 'MassifquantParam'
peakwidth(object)

## S4 replacement method for signature 'MassifquantParam'
peakwidth(object) <- value

## S4 method for signature 'MassifquantParam'
snthresh(object)

## S4 replacement method for signature 'MassifquantParam'
snthresh(object) <- value

## S4 method for signature 'MassifquantParam'
prefilter(object)

## S4 replacement method for signature 'MassifquantParam'
prefilter(object) <- value

## S4 method for signature 'MassifquantParam'
mzCenterFun(object)

## S4 replacement method for signature 'MassifquantParam'
mzCenterFun(object) <- value

## S4 method for signature 'MassifquantParam'
integrate(f)

## S4 replacement method for signature 'MassifquantParam'
integrate(object) <- value

## S4 method for signature 'MassifquantParam'
mzdiff(object)

## S4 replacement method for signature 'MassifquantParam'
mzdiff(object) <- value

## S4 method for signature 'MassifquantParam'
fitgauss(object)

## S4 replacement method for signature 'MassifquantParam'
fitgauss(object) <- value

## S4 method for signature 'MassifquantParam'
```

```
noise(object)

## S4 replacement method for signature 'MassifquantParam'
noise(object) <- value

## S4 method for signature 'MassifquantParam'
verboseColumns(object)

## S4 replacement method for signature 'MassifquantParam'
verboseColumns(object) <- value

## S4 method for signature 'MassifquantParam'
criticalValue(object)

## S4 replacement method for signature 'MassifquantParam'
criticalValue(object) <- value

## S4 method for signature 'MassifquantParam'
consecMissedLimit(object)

## S4 replacement method for signature 'MassifquantParam'
consecMissedLimit(object) <- value

## S4 method for signature 'MassifquantParam'
unions(object)

## S4 replacement method for signature 'MassifquantParam'
unions(object) <- value

## S4 method for signature 'MassifquantParam'
checkBack(object)

## S4 replacement method for signature 'MassifquantParam'
checkBack(object) <- value

## S4 method for signature 'MassifquantParam'
withWave(object)

## S4 replacement method for signature 'MassifquantParam'
withWave(object) <- value
```

Arguments

ppm	numeric(1) defining the maximal tolerated m/z deviation in consecutive scans in parts per million (ppm) for the initial ROI definition.
peakwidth	numeric(2). Only the first element is used by massifquant, which specifices the minimum peak length in time scans. For withWave = TRUE the second argument represents the maximum peak length subject to being greater than the mininum peak length (see also documentation of do_findChromPeaks_centWave).
snthresh	numeric(1) defining the signal to noise ratio cutoff.
prefilter	numeric(2). The first argument is only used if (withWave = TRUE); see findChromPeaks-centWave for details. The second argument specifies the min-

imum threshold for the maximum intensity of a chromatographic peak that must be met.

`mzCenterFun` Name of the function to calculate the m/z center of the chromatographic peak. Allowed are: `"wMean"`: intensity weighted mean of the peak's m/z values, `"mean"`: mean of the peak's m/z values, `"apex"`: use the m/z value at the peak apex, `"wMeanApex3"`: intensity weighted mean of the m/z value at the peak apex and the m/z values left and right of it and `"meanApex3"`: mean of the m/z value of the peak apex and the m/z values left and right of it.

`integrate` Integration method. For `integrate = 1` peak limits are found through descent on the mexican hat filtered data, for `integrate = 2` the descent is done on the real data. The latter method is more accurate but prone to noise, while the former is more robust, but less exact.

`mzdiff` `numeric(1)` representing the minimum difference in m/z dimension for peaks with overlapping retention times; can be negatove to allow overlap.

`fitgauss` `logical(1)` whether or not a Gaussian should be fitted to each peak.

`noise` `numeric(1)` allowing to set a minimum intensity required for centroids to be considered in the first analysis step (centroids with intensity < `noise` are omitted from ROI detection).

`verboseColumns` `logical(1)` whether additional peak meta data columns should be returned.

`criticalValue` `numeric(1)`. Suggested values: `(0.1-3.0)`. This setting helps determine the the Kalman Filter prediciton margin of error. A real centroid belonging to a bonafide peak must fall within the KF prediction margin of error. Much like in the construction of a confidence interval, `criticalVal` loosely translates to be a multiplier of the standard error of the prediction reported by the Kalman Filter. If the peak in the XC-MS sample have a small mass deviance in ppm error, a smaller critical value might be better and vice versa.

`consecMissedLimit`

`integer(1)` Suggested values: `(1,2,3)`. While a peak is in the proces of being detected by a Kalman Filter, the Kalman Filter may not find a predicted centroid in every scan. After 1 or more consecutive failed predictions, this setting informs Massifquant when to stop a Kalman Filter from following a candidate peak.

`unions` `integer(1)` set to `1` if apply t-test union on segmentation; set to `0` if no t-test to be applied on chromatographically continous peaks sharing same m/z range. Explanation: With very few data points, sometimes a Kalman Filter stops tracking a peak prematurely. Another Kalman Filter is instantiated and begins following the rest of the signal. Because tracking is done backwards to forwards, this algorithmic defect leaves a real peak divided into two segments or more. With this option turned on, the program identifies segmented peaks and combines them (merges them) into one with a two sample t-test. The potential danger of this option is that some truly distinct peaks may be merged.

`checkBack` `integer(1)` set to `1` if turned on; set to `0` if turned off. The convergence of a Kalman Filter to a peak's precise m/z mapping is very fast, but sometimes it incorporates erroneous centroids as part of a peak (especially early on). The `scanBack` option is an attempt to remove the occasional outlier that lies beyond the converged bounds of the Kalman Filter. The option does not directly affect identification of a peak because it is a postprocessing measure; it has not shown to be a extremely useful thus far and the default is set to being turned off.

`withWave` `logical(1)` if `TRUE`, the peaks identified first with Massifquant are subsequently filtered with the second step of the centWave algorithm, which includes wavelet estimation.

object	For findChromPeaks: an OnDiskMSnExp object containing the MS- and all other experiment-relevant data. For all other methods: a parameter object.
param	An MassifquantParam object containing all settings for the massifquant algorithm.
BPPARAM	A parameter class specifying if and how parallel processing should be performed. It defaults to bpparam. See documentation of the BiocParallel for more details. If parallel processing is enabled, peak detection is performed in parallel on several of the input samples.
return.type	Character specifying what type of object the method should return. Can be either "XCMSnExp" (default), "list" or "xcmsSet".
msLevel	integer(1) defining the MS level on which the peak detection should be performed. Defaults to msLevel = 1.
value	The value for the slot.
f	For integrate: a MassifquantParam object.

Details

This algorithm's performance has been tested rigorously on high resolution LC/OrbiTrap, TOF-MS data in centroid mode. Simultaneous kalman filters identify chromatographic peaks and calculate their area under the curve. The default parameters are set to operate on a complex LC-MS Orbitrap sample. Users will find it useful to do some simple exploratory data analysis to find out where to set a minimum intensity, and identify how many scans an average peak spans. The consecMissedLimit parameter has yielded good performance on Orbitrap data when set to (2) and on TOF data it was found best to be at (1). This may change as the algorithm has yet to be tested on many samples. The criticalValue parameter is perhaps most dificult to dial in appropriately and visual inspection of peak identification is the best suggested tool for quick optimization. The ppm and checkBack parameters have shown less influence than the other parameters and exist to give users flexibility and better accuracy.

Parallel processing (one process per sample) is supported and can be configured either by the BPPARAM parameter or by globally defining the parallel processing mode using the register method from the BiocParallel package.

Value

The MassifquantParam function returns a MassifquantParam class instance with all of the settings specified for chromatographic peak detection by the *massifquant* method.

For findChromPeaks: if return.type = "XCMSnExp" an XCMSnExp object with the results of the peak detection. If return.type = "list" a list of length equal to the number of samples with matrices specifying the identified peaks. If return.type = "xcmsSet" an xcmsSet object with the results of the peak detection.

Slots

.__classVersion__,ppm,peakwidth,snthresh,prefilter,mzCenterFun,integrate,mzdiff,fitgauss,noise,v
: See corresponding parameter above. .__classVersion__ stores the version from the class. Slots values should exclusively be accessed *via* the corresponding getter and setter methods listed above.

Note

These methods and classes are part of the updated and modernized xcms user interface which will eventually replace the findPeaks methods. It supports chromatographic peak detection on MSnExp and OnDiskMSnExp objects (both defined in the MSnbase package). All of the settings to the massifquant and centWave algorithm can be passed with a MassifquantParam object.

Author(s)

Christopher Conley, Johannes Rainer

References

Conley CJ, Smith R, Torgrip RJ, Taylor RM, Tautenhahn R and Prince JT "Massifquant: open-source Kalman filter-based XC-MS isotope trace feature detection" *Bioinformatics* 2014, 30(18):2636-43.

See Also

The do_findChromPeaks_massifquant core API function and findPeaks.massifquant for the old user interface.

XCMSnExp for the object containing the results of the peak detection.

Other peak detection methods: chromatographic-peak-detection, findChromPeaks-centWaveWithPredIsoROIs, findChromPeaks-centWave, findChromPeaks-matchedFilter, findPeaks-MSW

Examples

```
## Create a MassifquantParam object.
mqp <- MassifquantParam()
## Change snthresh parameter
snthresh(mqp) <- 30
mqp

## Perform the peak detection using massifquant on the files from the
## faahKO package. Files are read using the readMSData from the MSnbase
## package
library(faahKO)
library(MSnbase)
fls <- dir(system.file("cdf/KO", package = "faahKO"), recursive = TRUE,
           full.names = TRUE)
raw_data <- readMSData(fls[1:2], mode = "onDisk")
## Perform the peak detection using the settings defined above.
res <- findChromPeaks(raw_data, param = mqp)
head(chromPeaks(res))
```

---

findChromPeaks-matchedFilter

Peak detection in the chromatographic time domain

Description

The *matchedFilter* algorithm identifies peaks in the chromatographic time domain as described in [Smith 2006]. The intensity values are binned by cutting The LC/MS data into slices (bins) of a mass unit (`binSize` m/z) wide. Within each bin the maximal intensity is selected. The chromatographic peak detection is then performed in each bin by extending it based on the `steps` parameter to generate slices comprising bins `current_bin - steps +1` to `current_bin + steps - 1`. Each of these slices is then filtered with matched filtration using a second-derative Gaussian as the model peak shape. After filtration peaks are detected using a signal-to-ratio cut-off. For more details and illustrations see [Smith 2006].

The `MatchedFilterParam` class allows to specify all settings for a chromatographic peak detection using the matchedFilter method. Instances should be created with the `MatchedFilterParam` constructor.

The `findChromPeaks,OnDiskMSnExp,MatchedFilterParam` method performs peak detection using the *matchedFilter* algorithm on all samples from an `OnDiskMSnExp` object. `OnDiskMSnExp` objects encapsule all experiment specific data and load the spectra data (mz and intensity values) on the fly from the original files applying also all eventual data manipulations.

`binSize,binSize<-`: getter and setter for the `binSize` slot of the object.

`impute,impute<-`: getter and setter for the `impute` slot of the object.

`baseValue,baseValue<-`: getter and setter for the `baseValue` slot of the object.

`distance,distance<-`: getter and setter for the `distance` slot of the object.

`fwhm,fwhm<-`: getter and setter for the `fwhm` slot of the object.

`sigma,sigma<-`: getter and setter for the `sigma` slot of the object.

`max,max<-`: getter and setter for the `max` slot of the object.

`snthresh,snthresh<-`: getter and setter for the `snthresh` slot of the object.

`steps,steps<-`: getter and setter for the `steps` slot of the object.

`mzdiff,mzdiff<-`: getter and setter for the `mzdiff` slot of the object.

`index,index<-`: getter and setter for the `index` slot of the object.

Usage

```
MatchedFilterParam(binSize = 0.1, impute = "none", baseValue = numeric(),
  distance = numeric(), fwhm = 30, sigma = fwhm/2.3548, max = 5,
  snthresh = 10, steps = 2, mzdiff = 0.8 - binSize * steps,
  index = FALSE)

## S4 method for signature 'OnDiskMSnExp,MatchedFilterParam'
findChromPeaks(object, param,
  BPPARAM = bpparam(), return.type = "XCMSnExp", msLevel = 1L)

## S4 method for signature 'MatchedFilterParam'
show(object)

## S4 method for signature 'MatchedFilterParam'
binSize(object)

## S4 replacement method for signature 'MatchedFilterParam'
binSize(object) <- value
```

```
## S4 method for signature 'MatchedFilterParam'
impute(object)

## S4 replacement method for signature 'MatchedFilterParam'
impute(object) <- value

## S4 method for signature 'MatchedFilterParam'
baseValue(object)

## S4 replacement method for signature 'MatchedFilterParam'
baseValue(object) <- value

## S4 method for signature 'MatchedFilterParam'
distance(object)

## S4 replacement method for signature 'MatchedFilterParam'
distance(object) <- value

## S4 method for signature 'MatchedFilterParam'
fwhm(object)

## S4 replacement method for signature 'MatchedFilterParam'
fwhm(object) <- value

## S4 method for signature 'MatchedFilterParam'
sigma(object)

## S4 replacement method for signature 'MatchedFilterParam'
sigma(object) <- value

## S4 method for signature 'MatchedFilterParam'
max(x)

## S4 replacement method for signature 'MatchedFilterParam'
max(object) <- value

## S4 method for signature 'MatchedFilterParam'
snthresh(object)

## S4 replacement method for signature 'MatchedFilterParam'
snthresh(object) <- value

## S4 method for signature 'MatchedFilterParam'
steps(object)

## S4 replacement method for signature 'MatchedFilterParam'
steps(object) <- value

## S4 method for signature 'MatchedFilterParam'
mzdiff(object)

## S4 replacement method for signature 'MatchedFilterParam'
```

```
mzdiff(object) <- value

## S4 method for signature 'MatchedFilterParam'
index(object)

## S4 replacement method for signature 'MatchedFilterParam'
index(object) <- value
```

Arguments

binSize	numeric(1) specifying the width of the bins/slices in m/z dimension.
impute	Character string specifying the method to be used for missing value imputation. Allowed values are "none" (no linear interpolation), "lin" (linear interpolation), "linbase" (linear interpolation within a certain bin-neighborhood) and "intlin". See imputeLinInterpol for more details.
baseValue	The base value to which empty elements should be set. This is only considered for method = "linbase" and corresponds to the profBinLinBase's baselevel argument.
distance	For method = "linbase": number of non-empty neighboring element of an empty element that should be considered for linear interpolation. See details section for more information.
fwhm	numeric(1) specifying the full width at half maximum of matched filtration gaussian model peak. Only used to calculate the actual sigma, see below.
sigma	numeric(1) specifying the standard deviation (width) of the matched filtration model peak.
max	numeric(1) representing the maximum number of peaks that are expected/will be identified per slice.
snthresh	numeric(1) defining the signal to noise cutoff to be used in the chromatographic peak detection step.
steps	numeric(1) defining the number of bins to be merged before filtration (i.e. the number of neighboring bins that will be joined to the slice in which filtration and peak detection will be performed).
mzdiff	numeric(1) defining the minimum difference in m/z for peaks with overlapping retention times
index	logical(1) specifying whether indicies should be returned instead of values for m/z and retention times.
object	For findChromPeaks: an OnDiskMSnExp object containing the MS- and all other experiment-relevant data. For all other methods: a parameter object.
param	An MatchedFilterParam object containing all settings for the matchedFilter algorithm.
BPPARAM	A parameter class specifying if and how parallel processing should be performed. It defaults to bpparam. See documentation of the BiocParallel for more details. If parallel processing is enabled, peak detection is performed in parallel on several of the input samples.
return.type	Character specifying what type of object the method should return. Can be either "XCMSnExp" (default), "list" or "xcmsSet".
msLevel	integer(1) defining the MS level on which the peak detection should be performed. Defaults to msLevel = 1.

value	The value for the slot.
x	For max: a MatchedFilterParam object.

Details

The intensities are binned by the provided m/z values within each spectrum (scan). Binning is performed such that the bins are centered around the m/z values (i.e. the first bin includes all m/z values between min(mz) - bin_size/2 and min(mz) + bin_size/2).

For more details on binning and missing value imputation see binYonX and imputeLinInterpol methods.

Parallel processing (one process per sample) is supported and can be configured either by the BPPARAM parameter or by globally defining the parallel processing mode using the register method from the BiocParallel package.

Value

The MatchedFilterParam function returns a MatchedFilterParam class instance with all of the settings specified for chromatographic detection by the *matchedFilter* method.

For findChromPeaks: if return.type = "XCMSnExp" an XCMSnExp object with the results of the peak detection. If return.type = "list" a list of length equal to the number of samples with matrices specifying the identified peaks. If return.type = "xcmsSet" an xcmsSet object with the results of the peak detection.

Slots

.__classVersion__,binSize,impute,baseValue,distance,fwhm,sigma,max,snthresh,steps,mzdiff,index
: See corresponding parameter above. .__classVersion__ stores the version from the class. Slots values should exclusively be accessed *via* the corresponding getter and setter methods listed above.

Note

These methods and classes are part of the updated and modernized xcms user interface which will eventually replace the findPeaks methods. It supports chromatographic peak detection on MSnExp and OnDiskMSnExp objects (both defined in the MSnbase package). All of the settings to the matchedFilter algorithm can be passed with a MatchedFilterParam object.

Author(s)

Colin A Smith, Johannes Rainer

References

Colin A. Smith, Elizabeth J. Want, Grace O'Maille, Ruben Abagyan and Gary Siuzdak. "XCMS: Processing Mass Spectrometry Data for Metabolite Profiling Using Nonlinear Peak Alignment, Matching, and Identification" *Anal. Chem.* 2006, 78:779-787.

See Also

The do_findChromPeaks_matchedFilter core API function and findPeaks.matchedFilter for the old user interface.

XCMSnExp for the object containing the results of the chromatographic peak detection.

Other peak detection methods: chromatographic-peak-detection, findChromPeaks-centWaveWithPredIsoROIs, findChromPeaks-centWave, findChromPeaks-massifquant, findPeaks-MSW

Examples

```
## Create a MatchedFilterParam object. Note that we use a unnecessarily large
## binSize parameter to reduce the run-time of the example.
mfp <- MatchedFilterParam(binSize = 5)
## Change snthresh parameter
snthresh(mfp) <- 15
mfp

## Perform the peak detection using matchecFilter on the files from the
## faahKO package. Files are read using the readMSData from the MSnbase
## package
library(faahKO)
library(MSnbase)
fls <- dir(system.file("cdf/KO", package = "faahKO"), recursive = TRUE,
           full.names = TRUE)
raw_data <- readMSData(fls[1:2], mode = "onDisk")
## Perform the chromatographic peak detection using the settings defined
## above. Note that we are also disabling parallel processing in this
## example by registering a "SerialParam"
register(SerialParam())
res <- findChromPeaks(raw_data, param = mfp)
head(chromPeaks(res))
```

`findMZ` *Find fragment ions in xcmsFragment objects*

Description

This is a method to find a fragment mass with a ppm window in a xcmsFragment object

Usage

```
findMZ(object, find, ppmE=25, print=TRUE)
```

Arguments

`object`	xcmsFragment object type
`find`	The fragment ion to be found
`ppmE`	the ppm error window for searching
`print`	If we should print a nice little report

Details

The method simply searches for a given fragment ion in an xcmsFragment object type given a certain ppm error window

Value

A data frame with the following columns:

PrecursorMz	The precursor m/z of the fragment
MSnParentPeakID	An index ID of the location of the precursor peak in the xcmsFragment object
msLevel	The level of the found fragment ion
rt	the Retention time of the found ion
mz	the actual m/z of the found fragment ion
intensity	The intensity of the fragment ion
sample	Which sample the fragment ion came from
GroupPeakMSn	an ID if the peaks were grouped by an xcmsSet grouping
CollisionEnergy	The collision energy of the precursor scan

Author(s)

H. Paul Benton, <hpaul.beonton08@imperial.ac.uk>

References

H. Paul Benton, D.M. Wong, S.A.Strauger, G. Siuzdak "XCMS^2" Analytical Chemistry 2008

See Also

findneutral,

Examples

```
## Not run:
library(msdata)
mzdatapath <- system.file("iontrap", package = "msdata")
mzdatafiles<-list.files(mzdatapath, pattern = "extracted.mzData", recursive = TRUE, full.names = TRUE)
xs <- xcmsSet(mzdatafiles, method = "MS1")
##takes only one file from the file set
xfrag <- xcmsFragments(xs)
found<-findMZ(xfrag, 657.3433, 50)

## End(Not run)
```

---

findneutral *Find neutral losses in xcmsFragment objects*

Description

This is a method to find a neutral loss with a ppm window in a xcmsFragment object

Usage

```
findneutral(object, find, ppmE=25, print=TRUE)
```

Arguments

object	xcmsFragment object type
find	The neutral loss to be found
ppmE	the ppm error window for searching
print	If we should print a nice little report

Details

The method searches for a given neutral loss in an xcmsFragment object type given a certain ppm error window. The neutral losses are generated between neighbouring ions. The resulting data frame shows the whole scan in which the neutral loss was found.

Value

A data frame with the following columns:

PrecursorMz	The precursor m/z of the neutral losses
MSnParentPeakID	An index ID of the location of the precursor peak in the xcmsFragment object
msLevel	The level of the found fragment ion
rt	the Retention time of the found ion
mz	the actual m/z of the found fragment ion
intensity	The intensity of the fragment ion
sample	Which sample the fragment ion came from
GroupPeakMSn	an ID if the peaks were grouped by an xcmsSet grouping
CollisionEnergy	The collision energy of the precursor scan

Author(s)

H. Paul Benton, <hpbenton@scripps.edu>

References

H. Paul Benton, D.M. Wong, S.A.Strauger, G. Siuzdak "XCMS^2" Analytical Chemistry 2008

See Also

findMZ,

Examples

```
## Not run:
library(msdata)
mzdatapath <- system.file("iontrap", package = "msdata")
mzdatafiles<-list.files(mzdatapath, pattern = "extracted.mzData", recursive = TRUE, full.names = TRUE)
xs <- xcmsSet(mzdatafiles, method = "MS1")
##takes only one file from the file set
xfrag <- xcmsFragments(xs)
found<-findneutral(xfrag, 58.1455, 50)

## End(Not run)
```

`findPeaks-methods` *Feature detection for GC/MS and LC/MS Data - methods*

Description

A number of peak pickers exist in XCMS. `findPeaks` is the generic method.

Arguments

`object`	`xcmsRaw-class` object
`method`	Method to use for peak detection. See details.
`...`	Optional arguments to be passed along

Details

Different algorithms can be used by specifying them with the `method` argument. For example to use the matched filter approach described by Smith et al (2006) one would use: `findPeaks(object, method="matchedFilt` This is also the default.

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

A character vector of *nicknames* for the algorithms available is returned by `getOption("BioC")$xcms$findPeaks.meth` If the nickname of a method is called "centWave", the help page for that specific method can be accessed with `?findPeaks.centWave`.

Value

A matrix with columns:

`mz`	weighted (by intensity) mean of peak m/z across scans
`mzmin`	m/z of minimum step
`mzmax`	m/z of maximum step
`rt`	retention time of peak midpoint
`rtmin`	leading edge of peak retention time
`rtmax`	trailing edge of peak retention time
`into`	integrated area of original (raw) peak
`maxo`	maximum intensity of original (raw) peak

and additional columns depending on the choosen method.

Methods

object = "xcmsRaw" `findPeaks(object, ...)`

See Also

`findPeaks.matchedFilter` `findPeaks.centWave` `findPeaks.addPredictedIsotopeFeatures` `findPeaks.centWaveWithPredictedIsotopeROIs` `xcmsRaw-class`

findPeaks-MSW *Single-spectrum non-chromatography MS data peak detection*

Description

Perform peak detection in mass spectrometry direct injection spectrum using a wavelet based algorithm.

The MSWParam class allows to specify all settings for a peak detection using the MSW method. Instances should be created with the MSWParam constructor.

The findChromPeaks,OnDiskMSnExp,MSWParam method performs peak detection in single-spectrum non-chromatography MS data using functionality from the MassSpecWavelet package on all samples from an OnDiskMSnExp object. OnDiskMSnExp objects encapsule all experiment specific data and load the spectra data (mz and intensity values) on the fly from the original files applying also all eventual data manipulations.

snthresh,snthresh<-: getter and setter for the snthresh slot of the object.

verboseColumns,verboseColumns<-: getter and setter for the verboseColumns slot of the object.

scales,scales<-: getter and setter for the scales slot of the object.

nearbyPeak,nearbyPeak<-: getter and setter for the nearbyPeak slot of the object.

peakScaleRange,peakScaleRange<-: getter and setter for the peakScaleRange slot of the object.

ampTh,ampTh<-: getter and setter for the ampTh slot of the object.

minNoiseLevel,minNoiseLevel<-: getter and setter for the minNoiseLevel slot of the object.

ridgeLength,ridgeLength<-: getter and setter for the ridgeLength slot of the object.

peakThr,peakThr<-: getter and setter for the peakThr slot of the object.

tuneIn,tuneIn<-: getter and setter for the tuneIn slot of the object.

addParams,addParams<-: getter and setter for the addParams slot of the object. This slot stores optional additional parameters to be passed to the identifyMajorPeaks and sav.gol functions from the MassSpecWavelet package.

Usage

```
MSWParam(snthresh = 3, verboseColumns = FALSE, scales = c(1, seq(2, 30,
  2), seq(32, 64, 4)), nearbyPeak = TRUE, peakScaleRange = 5,
  ampTh = 0.01, minNoiseLevel = ampTh/snthresh, ridgeLength = 24,
  peakThr = NULL, tuneIn = FALSE, ...)

## S4 method for signature 'OnDiskMSnExp,MSWParam'
findChromPeaks(object, param,
  BPPARAM = bpparam(), return.type = "XCMSnExp", msLevel = 1L)

## S4 method for signature 'MSWParam'
show(object)

## S4 method for signature 'MSWParam'
snthresh(object)

## S4 replacement method for signature 'MSWParam'
```

```
snthresh(object) <- value

## S4 method for signature 'MSWParam'
verboseColumns(object)

## S4 replacement method for signature 'MSWParam'
verboseColumns(object) <- value

## S4 method for signature 'MSWParam'
scales(object)

## S4 replacement method for signature 'MSWParam'
scales(object) <- value

## S4 method for signature 'MSWParam'
nearbyPeak(object)

## S4 replacement method for signature 'MSWParam'
nearbyPeak(object) <- value

## S4 method for signature 'MSWParam'
peakScaleRange(object)

## S4 replacement method for signature 'MSWParam'
peakScaleRange(object) <- value

## S4 method for signature 'MSWParam'
ampTh(object)

## S4 replacement method for signature 'MSWParam'
ampTh(object) <- value

## S4 method for signature 'MSWParam'
minNoiseLevel(object)

## S4 replacement method for signature 'MSWParam'
minNoiseLevel(object) <- value

## S4 method for signature 'MSWParam'
ridgeLength(object)

## S4 replacement method for signature 'MSWParam'
ridgeLength(object) <- value

## S4 method for signature 'MSWParam'
peakThr(object)

## S4 replacement method for signature 'MSWParam'
peakThr(object) <- value

## S4 method for signature 'MSWParam'
tuneIn(object)
```

```
## S4 replacement method for signature 'MSWParam'
tuneIn(object) <- value

## S4 method for signature 'MSWParam'
addParams(object)

## S4 replacement method for signature 'MSWParam'
addParams(object) <- value
```

Arguments

snthresh	numeric(1) defining the signal to noise ratio cutoff.
verboseColumns	logical(1) whether additional peak meta data columns should be returned.
scales	Numeric defining the scales of the continuous wavelet transform (CWT).
nearbyPeak	logical(1) whether to include nearby peaks of major peaks.
peakScaleRange	numeric(1) defining the scale range of the peak (larger than 5 by default).
ampTh	numeric(1) defining the minimum required relative amplitude of the peak (ratio of the maximum of CWT coefficients).
minNoiseLevel	numeric(1) defining the minimum noise level used in computing the SNR.
ridgeLength	numeric(1) defining the minimum highest scale of the peak in 2-D CWT coefficient matrix.
peakThr	numeric(1) with the minimum absolute intensity (above baseline) of peaks to be picked. If provided, the smoothing function sav.gol function is called to estimate the local intensity.
tuneIn	logical(1) whther to tune in the parameter estimation of the detected peaks.
...	Additional parameters to be passed to the identifyMajorPeaks and sav.gol functions from the MassSpecWavelet package.
object	For findChromPeaks: an OnDiskMSnExp object containing the MS- and all other experiment-relevant data. For all other methods: a parameter object.
param	An MSWParam object containing all settings for the algorithm.
BPPARAM	A parameter class specifying if and how parallel processing should be performed. It defaults to bpparam. See documentation of the BiocParallel for more details. If parallel processing is enabled, peak detection is performed in parallel on several of the input samples.
return.type	Character specifying what type of object the method should return. Can be either "XCMSnExp" (default), "list" or "xcmsSet".
msLevel	integer(1) defining the MS level on which the peak detection should be performed. Defaults to msLevel = 1.
value	The value for the slot.

Details

This is a wrapper for the peak picker in Bioconductor's MassSpecWavelet package calling peakDetectionCWT and tuneInPeakInfo functions. See the *xcmsDirect* vignette for more information.

Parallel processing (one process per sample) is supported and can be configured either by the BPPARAM parameter or by globally defining the parallel processing mode using the register method from the BiocParallel package.

Value

The MSWParam function returns a MSWParam class instance with all of the settings specified for peak detection by the *MSW* method.

For findChromPeaks: if return.type = "XCMSnExp" an XCMSnExp object with the results of the peak detection. If return.type = "list" a list of length equal to the number of samples with matrices specifying the identified peaks. If return.type = "xcmsSet" an xcmsSet object with the results of the detection.

Slots

.__classVersion__,snthresh,verboseColumns,scales,nearbyPeak,peakScaleRange,ampTh,minNoiseLevel,r
: See corresponding parameter above. .__classVersion__ stores the version from the class. Slots values should exclusively be accessed *via* the corresponding getter and setter methods listed above.

Note

These methods and classes are part of the updated and modernized xcms user interface which will eventually replace the findPeaks methods. It supports peak detection on MSnExp and OnDiskMSnExp objects (both defined in the MSnbase package). All of the settings to the algorithm can be passed with a MSWParam object.

Author(s)

Joachim Kutzera, Steffen Neumann, Johannes Rainer

See Also

The do_findPeaks_MSW core API function and findPeaks.MSW for the old user interface.

XCMSnExp for the object containing the results of the peak detection.

Other peak detection methods: chromatographic-peak-detection, findChromPeaks-centWaveWithPredIsoROIs, findChromPeaks-centWave, findChromPeaks-massifquant, findChromPeaks-matchedFilter

Examples

```
## Create a MSWParam object
mp <- MSWParam()
## Change snthresh parameter
snthresh(mp) <- 15
mp

## Loading a small subset of direct injection, single spectrum files
library(msdata)
fticrf <- list.files(system.file("fticr", package = "msdata"),
                     recursive = TRUE, full.names = TRUE)
fticr <- readMSData(fticrf[1:2], msLevel. = 1, mode = "onDisk")

## Perform the MSW peak detection on these:
p <- MSWParam(scales = c(1, 7), peakThr = 80000, ampTh = 0.005,
              SNR.method = "data.mean", winSize.noise = 500)
fticr <- findChromPeaks(fticr, param = p)

head(chromPeaks(fticr))
```

`findPeaks.addPredictedIsotopeFeatures-methods`
Feature detection based on predicted isotope features for high resolution LC/MS data

Description

Peak density and wavelet based feature detection aiming at isotope peaks for high resolution LC/MS data in centroid mode

Arguments

`object`	`xcmsSet` object
`ppm`	maxmial tolerated m/z deviation in consecutive scans, in ppm (parts per million)
`peakwidth`	Chromatographic peak width, given as range (min,max) in seconds
`prefilter`	`prefilter=c(k,I)`. Prefilter step for the first phase. Mass traces are only retained if they contain at least `k` peaks with intensity >= `I`.
`mzCenterFun`	Function to calculate the m/z center of the feature: `wMean` intensity weighted mean of the feature m/z values, `mean` mean of the feature m/z values, `apex` use m/z value at peak apex, `wMeanApex3` intensity weighted mean of the m/z value at peak apex and the m/z value left and right of it, `meanApex3` mean of the m/z value at peak apex and the m/z value left and right of it.
`integrate`	Integration method. If `=1` peak limits are found through descent on the mexican hat filtered data, if `=2` the descent is done on the real data. Method 2 is very accurate but prone to noise, while method 1 is more robust to noise but less exact.
`mzdiff`	minimum difference in m/z for peaks with overlapping retention times, can be negative to allow overlap
`fitgauss`	logical, if TRUE a Gaussian is fitted to each peak
`scanrange`	scan range to process
`noise`	optional argument which is useful for data that was centroided without any intensity threshold, centroids with intensity < `noise` are omitted from ROI detection
`sleep`	number of seconds to pause between plotting peak finding cycles
`verbose.columns`	logical, if TRUE additional peak meta data columns are returned
`xcmsPeaks`	peak list picked using the `centWave` algorithm with parameter `verbose.columns` set to TRUE (columns `scmin` and `scmax` needed)
`snthresh`	signal to noise ratio cutoff, definition see below.
`maxcharge`	max. number of the isotope charge.
`maxiso`	max. number of the isotope peaks to predict for each detected feature.
`mzIntervalExtension`	logical, if TRUE predicted isotope ROIs (regions of interest) are extended in the m/z dimension to increase the detection of low intensity and hence noisy peaks.

Details

This algorithm is most suitable for high resolution LC/{TOF,OrbiTrap,FTICR}-MS data in centroid mode. In the first phase of the method isotope ROIs (regions of interest) in the LC/MS map are predicted. In the second phase these mass traces are further analysed. Continuous wavelet transform (CWT) is used to locate chromatographic peaks on different scales. The resulting peak list and the given peak list (`xcmsPeaks`) are merged and redundant peaks are removed.

Value

A matrix with columns:

`mz`	weighted (by intensity) mean of peak m/z across scans
`mzmin`	m/z peak minimum
`mzmax`	m/z peak maximum
`rt`	retention time of peak midpoint
`rtmin`	leading edge of peak retention time
`rtmax`	trailing edge of peak retention time
`into`	integrated peak intensity
`intb`	baseline corrected integrated peak intensity
`maxo`	maximum peak intensity
`sn`	Signal/Noise ratio, defined as `(maxo - baseline)/sd`, where `maxo` is the maximum peak intensity, `baseline` the estimated baseline value and `sd` the standard deviation of local chromatographic noise.
`egauss`	RMSE of Gaussian fit
	if `verbose.columns` is `TRUE` additionally :
`mu`	Gaussian parameter mu
`sigma`	Gaussian parameter sigma
`h`	Gaussian parameter h
`f`	Region number of m/z ROI where the peak was localised
`dppm`	m/z deviation of mass trace across scans in ppm
`scale`	Scale on which the peak was localised
`scpos`	Peak position found by wavelet analysis
`scmin`	Left peak limit found by wavelet analysis (scan number)
`scmax`	Right peak limit found by wavelet analysis (scan number)

Methods

object = "xcmsRaw" `findPeaks.centWave(object, ppm=25, peakwidth=c(20,50), prefilter=c(3,10`

Author(s)

Ralf Tautenhahn

References

Ralf Tautenhahn, Christoph B\"ottcher, and Steffen Neumann "Highly sensitive feature detection for high resolution LC/MS" BMC Bioinformatics 2008, 9:504\ 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

findPeaks.centWave findPeaks-methods xcmsRaw-class

---

findPeaks.centWave-methods

Feature detection for high resolution LC/MS data

Description

Peak density and wavelet based feature detection for high resolution LC/MS data in centroid mode

Arguments

object	xcmsSet object
ppm	maxmial tolerated m/z deviation in consecutive scans, in ppm (parts per million)
peakwidth	Chromatographic peak width, given as range (min,max) in seconds
snthresh	signal to noise ratio cutoff, definition see below.
prefilter	prefilter=c(k,I). Prefilter step for the first phase. Mass traces are only retained if they contain at least k peaks with intensity >= I.
mzCenterFun	Function to calculate the m/z center of the feature: wMean intensity weighted mean of the feature m/z values, mean mean of the feature m/z values, apex use m/z value at peak apex, wMeanApex3 intensity weighted mean of the m/z value at peak apex and the m/z value left and right of it, meanApex3 mean of the m/z value at peak apex and the m/z value left and right of it.
integrate	Integration method. If =1 peak limits are found through descent on the mexican hat filtered data, if =2 the descent is done on the real data. Method 2 is very accurate but prone to noise, while method 1 is more robust to noise but less exact.
mzdiff	minimum difference in m/z for peaks with overlapping retention times, can be negative to allow overlap
fitgauss	logical, if TRUE a Gaussian is fitted to each peak
scanrange	scan range to process
noise	optional argument which is useful for data that was centroided without any intensity threshold, centroids with intensity < noise are omitted from ROI detection
sleep	number of seconds to pause between plotting peak finding cycles
verbose.columns	logical, if TRUE additional peak meta data columns are returned

ROI.list	A optional list of ROIs that represents detected mass traces (ROIs). If this list is empty (default) then centWave detects the mass trace ROIs, otherwise this step is skipped and the supplied ROIs are used in the peak detection phase. Each ROI object in the list has the following slots: scmin start scan index, scmax end scan index, mzmin minimum m/z, mzmax maximum m/z, length number of scans, intensity summed intensity.
firstBaselineCheck	logical, if TRUE continuous data within ROI is checked to be above 1st baseline
roiScales	numeric, optional vector of scales for each ROI in ROI.list to be used for the centWave-wavelets

Details

This algorithm is most suitable for high resolution LC/{TOF,OrbiTrap,FTICR}-MS data in centroid mode. In the first phase of the method mass traces (characterised as regions with less than ppm m/z deviation in consecutive scans) in the LC/MS map are located. In the second phase these mass traces are further analysed. Continuous wavelet transform (CWT) is used to locate chromatographic peaks on different scales.

Value

A matrix with columns:

mz	weighted (by intensity) mean of peak m/z across scans
mzmin	m/z peak minimum
mzmax	m/z peak maximum
rt	retention time of peak midpoint
rtmin	leading edge of peak retention time
rtmax	trailing edge of peak retention time
into	integrated peak intensity
intb	baseline corrected integrated peak intensity
maxo	maximum peak intensity
sn	Signal/Noise ratio, defined as (maxo - baseline)/sd, where maxo is the maximum peak intensity, baseline the estimated baseline value and sd the standard deviation of local chromatographic noise.
egauss	RMSE of Gaussian fit
	if verbose.columns is TRUE additionally :
mu	Gaussian parameter mu
sigma	Gaussian parameter sigma
h	Gaussian parameter h
f	Region number of m/z ROI where the peak was localised
dppm	m/z deviation of mass trace across scans in ppm
scale	Scale on which the peak was localised
scpos	Peak position found by wavelet analysis
scmin	Left peak limit found by wavelet analysis (scan number)
scmax	Right peak limit found by wavelet analysis (scan number)

Methods

object = "xcmsRaw" `findPeaks.centWave(object, ppm=25, peakwidth=c(20,50), snthresh=10, pref`

Author(s)

Ralf Tautenhahn

References

Ralf Tautenhahn, Christoph B\"ottcher, and Steffen Neumann "Highly sensitive feature detection for high resolution LC/MS" BMC Bioinformatics 2008, 9:504

See Also

`centWave` for the new user interface. `findPeaks-methods` `xcmsRaw-class`

---

findPeaks.centWaveWithPredictedIsotopeROIs-methods

Feature detection with centWave and additional isotope features

---

Description

Peak density and wavelet based feature detection for high resolution LC/MS data in centroid mode with additional peak picking of isotope features on basis of isotope peak predictions

Arguments

`object`	`xcmsSet` object
`ppm`	maxmial tolerated m/z deviation in consecutive scans, in ppm (parts per million)
`peakwidth`	Chromatographic peak width, given as range (min,max) in seconds
`snthresh`	signal to noise ratio cutoff, definition see below.
`prefilter`	`prefilter=c(k,I)`. Prefilter step for the first phase. Mass traces are only retained if they contain at least `k` peaks with intensity >= `I`.
`mzCenterFun`	Function to calculate the m/z center of the feature: `wMean` intensity weighted mean of the feature m/z values, `mean` mean of the feature m/z values, `apex` use m/z value at peak apex, `wMeanApex3` intensity weighted mean of the m/z value at peak apex and the m/z value left and right of it, `meanApex3` mean of the m/z value at peak apex and the m/z value left and right of it.
`integrate`	Integration method. If `=1` peak limits are found through descent on the mexican hat filtered data, if `=2` the descent is done on the real data. Method 2 is very accurate but prone to noise, while method 1 is more robust to noise but less exact.
`mzdiff`	minimum difference in m/z for peaks with overlapping retention times, can be negative to allow overlap
`fitgauss`	logical, if TRUE a Gaussian is fitted to each peak
`scanrange`	scan range to process

noise	optional argument which is useful for data that was centroided without any intensity threshold, centroids with intensity < noise are omitted from ROI detection
sleep	number of seconds to pause between plotting peak finding cycles
verbose.columns	logical, if TRUE additional peak meta data columns are returned
ROI.list	A optional list of ROIs that represents detected mass traces (ROIs). If this list is empty (default) then centWave detects the mass trace ROIs, otherwise this step is skipped and the supplied ROIs are used in the peak detection phase. Each ROI object in the list has the following slots: scmin start scan index, scmax end scan index, mzmin minimum m/z, mzmax maximum m/z, length number of scans, intensity summed intensity.
firstBaselineCheck	logical, if TRUE continuous data within ROI is checked to be above 1st baseline
roiScales	numeric, optional vector of scales for each ROI in ROI.list to be used for the centWave-wavelets
snthreshIsoROIs	signal to noise ratio cutoff for predicted isotope ROIs, definition see below.
maxcharge	max. number of the isotope charge.
maxiso	max. number of the isotope peaks to predict for each detected feature.
mzIntervalExtension	logical, if TRUE predicted isotope ROIs (regions of interest) are extended in the m/z dimension to increase the detection of low intensity and hence noisy peaks.

Details

This algorithm is most suitable for high resolution LC/{TOF,OrbiTrap,FTICR}-MS data in centroid mode. The centWave algorithm is applied in two peak picking steps as follows. In the first peak picking step ROIs (regions of interest, characterised as regions with less than ppm m/z deviation in consecutive scans) in the LC/MS map are located and further analysed using continuous wavelet transform (CWT) for the localization of chromatographic peaks on different scales. In the second peak picking step isotope ROIs in the LC/MS map are predicted further analysed using continuous wavelet transform (CWT) for the localization of chromatographic peaks on different scales. The peak lists resulting from both peak picking steps are merged and redundant peaks are removed.

Value

A matrix with columns:

mz	weighted (by intensity) mean of peak m/z across scans
mzmin	m/z peak minimum
mzmax	m/z peak maximum
rt	retention time of peak midpoint
rtmin	leading edge of peak retention time
rtmax	trailing edge of peak retention time
into	integrated peak intensity
intb	baseline corrected integrated peak intensity
maxo	maximum peak intensity

sn	Signal/Noise ratio, defined as (maxo - baseline)/sd, where maxo is the maximum peak intensity, baseline the estimated baseline value and sd the standard deviation of local chromatographic noise.
egauss	RMSE of Gaussian fit
	if verbose.columns is TRUE additionally :
mu	Gaussian parameter mu
sigma	Gaussian parameter sigma
h	Gaussian parameter h
f	Region number of m/z ROI where the peak was localised
dppm	m/z deviation of mass trace across scans in ppm
scale	Scale on which the peak was localised
scpos	Peak position found by wavelet analysis
scmin	Left peak limit found by wavelet analysis (scan number)
scmax	Right peak limit found by wavelet analysis (scan number)

Methods

object = "xcmsRaw" `findPeaks.centWaveWithPredictedIsotopeROIs(object, ppm=25, peakwidth=c(20`

Author(s)

Ralf Tautenhahn

References

Ralf Tautenhahn, Christoph B\"ottcher, and Steffen Neumann "Highly sensitive feature detection for high resolution LC/MS" BMC Bioinformatics 2008, 9:504\ 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

do_findChromPeaks_centWaveWithPredIsoROIs for the corresponding core API function. findPeaks.addPredicted findPeaks.centWave findPeaks-methods xcmsRaw-class

---

findPeaks.massifquant-methods

Feature detection for XC-MS data.

Description

Massifquant is a Kalman filter (KF) based feature detection for XC-MS data in centroid mode (currently in experimental stage). Optionally allows for calling the method "centWave" on features discovered by Massifquant to further refine the feature detection; to do so, supply any additional parameters specific to centWave (even more experimental). The method may be conveniently called through the xcmsSet(...) method.

Arguments

	The following arguments are specific to Massifquant. Any additional arguments supplied must correspond as specified by the method findPeaks.centWave.
object	An xcmsRaw object.
criticalValue	Numeric: Suggested values: (0.1-3.0). This setting helps determine the the Kalman Filter prediciton margin of error. A real centroid belonging to a bonafide feature must fall within the KF prediction margin of error. Much like in the construction of a confidence interval, criticalVal loosely translates to be a multiplier of the standard error of the prediction reported by the Kalman Filter. If the features in the XC-MS sample have a small mass deviance in ppm error, a smaller critical value might be better and vice versa.
consecMissedLimit	Integer: Suggested values:(1,2,3). While a feature is in the proces of being detected by a Kalman Filter, the Kalman Filter may not find a predicted centroid in every scan. After 1 or more consecutive failed predictions, this setting informs Massifquant when to stop a Kalman Filter from following a candidate feature.
prefilter	Numeric Vector: (Positive Integer, Positive Numeric): The first argument is only used if (withWave = 1); see centWave for details. The second argument specifies the minimum threshold for the maximum intensity of a feature that must be met.
peakwidth	Integer Vector: (Positive Integer, Positive Integer): Only the first argument is used for Massifquant, which specifices the minimum feature length in time scans. If centWave is used, then the second argument is the maximum feature length subject to being greater than the mininum feature length.
ppm	The minimum estimated parts per million mass resolution a feature must possess.
unions	Integer: set to 1 if apply t-test union on segmentation; set to 0 if no t-test to be applied on chromatographically continous features sharing same m/z range. Explanation: With very few data points, sometimes a Kalman Filter stops tracking a feature prematurely. Another Kalman Filter is instantiated and begins following the rest of the signal. Because tracking is done backwards to forwards, this algorithmic defect leaves a real feature divided into two segments or more. With this option turned on, the program identifies segmented features and combines them (merges them) into one with a two sample t-test. The potential danger of this option is that some truly distinct features may be merged.
withWave	Integer: set to 1 if turned on; set to 0 if turned off. Allows the user to find features first with Massifquant and then filter those features with the second phase of centWave, which includes wavelet estimation.
checkBack	Integer: set to 1 if turned on; set to 0 if turned off. The convergence of a Kalman Filter to a feature's precise m/z mapping is very fast, but sometimes it incorporates erroneous centroids as part of a feature (especially early on). The "scanBack" option is an attempt to remove the occasional outlier that lies beyond the converged bounds of the Kalman Filter. The option does not directly affect identification of a feature because it is a postprocessing measure; it has not shown to be a extremely useful thus far and the default is set to being turned off.

Details

This algorithm's performance has been tested rigorously on high resolution LC/{OrbiTrap, TOF}-MS data in centroid mode. Simultaneous kalman filters identify features and calculate their area

under the curve. The default parameters are set to operate on a complex LC-MS Orbitrap sample. Users will find it useful to do some simple exploratory data analysis to find out where to set a minimum intensity, and identify how many scans an average feature spans. The "consecMissedLimit" parameter has yielded good performance on Orbitrap data when set to (2) and on TOF data it was found best to be at (1). This may change as the algorithm has yet to be tested on many samples. The "criticalValue" parameter is perhaps most dificult to dial in appropriately and visual inspection of peak identification is the best suggested tool for quick optimization. The "ppm" and "checkBack" parameters have shown less influence than the other parameters and exist to give users flexibility and better accuracy.

Value

If the method findPeaks.massifquant(...) is used, then a matrix is returned with rows corresponding to features, and properties of the features listed with the following column names. Otherwise, if centWave feature is used also (withWave = 1), or Massifquant is called through the xcmsSet(...) method, then their corresponding return values are used.

`mz`	weighted m/z mean (weighted by intensity) of the feature
`mzmin`	m/z lower boundary of the feature
`mzmax`	m/z upper boundary of the feature
`rtmin`	starting scan time of the feature
`rtmax`	starting scan time of the feature
`into`	the raw quantitation (area under the curve) of the feature.
`area`	feature area that is not normalized by the scan rate.

Methods

object = "xcmsRaw" `findPeaks.massifquant(object, ppm=10, peakwidth=c(20,50), snthresh=10,  pre`

Author(s)

Christopher Conley

References

Submitted for review. Christopher Conley, Ralf J .O Torgrip. Ryan Taylor, and John T. Prince. "Massifquant: open-source Kalman filter based XC-MS feature detection". August 2013.

See Also

`centWave` for the new user interface. `findPeaks-methods` `xcmsSet` `xcmsRaw` `xcmsRaw-class`

Examples

```
library(faahKO)
library(xcms)
#load all the wild type and Knock out samples
cdfpath <- system.file("cdf", package = "faahKO")
## Subset to only the first 2 files.
cdffiles <- list.files(cdfpath, recursive = TRUE, full.names = TRUE)[1:2]

## Run the massifquant analysis. Setting the noise level to 10000 to speed up
```

```
## execution of the examples - in a real use case it should be set to a reasoable
## value.
xset <- xcmsSet(cdffiles, method = "massifquant",
                consecMissedLimit = 1,
                snthresh = 10,
                criticalValue = 1.73,
                ppm = 10,
                peakwidth= c(30, 60),
                prefilter= c(1,3000),
                noise = 10000,
                withWave = 0)
```

`findPeaks.matchedFilter,xcmsRaw-method`
Peak detection in the chromatographic time domain

Description

Find peaks in the chromatographic time domain of the profile matrix. For more details see do_findChromPeaks_matched

Usage

```
## S4 method for signature 'xcmsRaw'
findPeaks.matchedFilter(object, fwhm = 30,
  sigma = fwhm/2.3548, max = 5, snthresh = 10, step = 0.1, steps = 2,
  mzdiff = 0.8 - step * steps, index = FALSE, sleep = 0,
  scanrange = numeric())
```

Arguments

`object`	The `xcmsRaw` object on which peak detection should be performed.
`fwhm`	`numeric(1)` specifying the full width at half maximum of matched filtration gaussian model peak. Only used to calculate the actual sigma, see below.
`sigma`	`numeric(1)` specifying the standard deviation (width) of the matched filtration model peak.
`max`	`numeric(1)` representing the maximum number of peaks that are expected/will be identified per slice.
`snthresh`	`numeric(1)` defining the signal to noise cutoff to be used in the chromatographic peak detection step.
`step`	numeric(1) specifying the width of the bins/slices in m/z dimension.
`steps`	`numeric(1)` defining the number of bins to be merged before filtration (i.e. the number of neighboring bins that will be joined to the slice in which filtration and peak detection will be performed).
`mzdiff`	`numeric(1)` defining the minimum difference in m/z for peaks with overlapping retention times
`index`	`logical(1)` specifying whether indicies should be returned instead of values for m/z and retention times.
`sleep`	(DEPRECATED). The use of this parameter is highly discouraged, as it could cause problems in parallel processing mode.
`scanrange`	Numeric vector defining the range of scans to which the original `object` should be sub-setted before peak detection.

Value

A matrix, each row representing an intentified chromatographic peak, with columns:

mz Intensity weighted mean of m/z values of the peak across scans.

mzmin Minimum m/z of the peak.

mzmax Maximum m/z of the peak.

rt Retention time of the peak's midpoint.

rtmin Minimum retention time of the peak.

rtmax Maximum retention time of the peak.

into Integrated (original) intensity of the peak.

intf Integrated intensity of the filtered peak.

maxo Maximum intensity of the peak.

maxf Maximum intensity of the filtered peak.

i Rank of peak in merged EIC (`<= max`).

sn Signal to noise ratio of the peak.

Author(s)

Colin A. Smith

References

Colin A. Smith, Elizabeth J. Want, Grace O'Maille, Ruben Abagyan and Gary Siuzdak. "XCMS: Processing Mass Spectrometry Data for Metabolite Profiling Using Nonlinear Peak Alignment, Matching, and Identification" *Anal. Chem.* 2006, 78:779-787. @family Old peak detection methods

See Also

`matchedFilter` for the new user interface. `xcmsRaw`, `do_findChromPeaks_matchedFilter` for the core function performing the peak detection.

`findPeaks.MS1-methods` *Collecting MS1 precursor peaks*

Description

Collecting Tandem MS or MS^n Mass Spectrometry precursor peaks as annotated in XML raw file

Arguments

`object`	`xcmsRaw` object

Details

Some mass spectrometers can acquire MS1 and MS2 (or MS^n scans) quasi simultaneously, e.g. in data dependent tandem MS or DDIT mode.

Since xcmsFragments attaches *all* MS^n peaks to MS1 peaks in xcmsSet, it is important that findPeaks and xcmsSet do not miss any MS1 precursor peak.

To be sure that all MS1 precursor peaks are in an xcmsSet, findPeaks.MS1 does not do an actual peak picking, but simply uses the annotation stored in mzXML, mzData or mzML raw files.

This relies on the following XML tags:

mzData:

```
<spectrum id="463"> <spectrumInstrument msLevel="2">
<cvParam cvLabel="psi" accession="PSI:1000039" name="TimeInSeconds" value="92.7743"/>
</spectrumInstrument> <precursor msLevel="1" spectrumRef="461">
<cvParam cvLabel="psi" accession="PSI:1000040" name="MassToChargeRatio" value="462.091"/>
<cvParam cvLabel="psi" accession="PSI:1000042" name="Intensity" value="366.674"/>
</precursor> </spectrum>
```

mzXML:

```
<scan num="17" msLevel="2" retentionTime="PT1.5224S"> <precursorMz precursorInte
</scan>
```

Several mzXML and mzData converters are known to create incomplete files, either without intensities (they will be set to 0) or without the precursor retention time (then a reasonably close rt will be chosen. NYI).

Value

A matrix with columns:

`mz, mzmin, mzmax`
: annotated MS1 precursor selection mass

`rt, rtmin, rtmax`
: annotated MS1 precursor retention time

`into, maxo, sn`
: annotated MS1 precursor intensity

Methods

object = "xcmsRaw" `findPeaks.MS1(object)`

Author(s)

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

See Also

findPeaks-methods xcmsRaw-class

`findPeaks.MSW,xcmsRaw-method`
Peak detection for single-spectrum non-chromatography MS data

Description

This method performs peak detection in mass spectrometry direct injection spectrum using a wavelet based algorithm.

Usage

```
## S4 method for signature 'xcmsRaw'
findPeaks.MSW(object, snthresh = 3,
  verbose.columns = FALSE, ...)
```

Arguments

`object`	The `xcmsRaw` object on which peak detection should be performed.
`snthresh`	`numeric(1)` defining the signal to noise ratio cutoff.
`verbose.columns`	Logical whether additional peak meta data columns should be returned.
`...`	Additional parameters to be passed to the `identifyMajorPeaks` and `sav.gol` functions from the `MassSpecWavelet` package.

Details

This is a wrapper around the peak picker in Bioconductor's `MassSpecWavelet` package calling `peakDetectionCWT` and `tuneInPeakInfo` functions.

Value

A matrix, each row representing an intentified peak, with columns:

mz m/z value of the peak at the centroid position.

mzmin Minimum m/z of the peak.

mzmax Maximum m/z of the peak.

rt Always `-1`.

rtmin Always `-1`.

rtmax Always `-1`.

into Integrated (original) intensity of the peak.

maxo Maximum intensity of the peak.

intf Always `NA`.

maxf Maximum MSW-filter response of the peak.

sn Signal to noise ratio.

Author(s)

Joachim Kutzera, Steffen Neumann, Johannes Rainer

See Also

MSW for the new user interface, do_findPeaks_MSW for the downstream analysis function or peakDetectionCWT from the MassSpecWavelet for details on the algorithm and additionally supported parameters.

GenericParam-class *Generic parameter class*

Description

The GenericParam class allows to store generic parameter information such as the name of the function that was/has to be called (slot fun) and its arguments (slot args). This object is used to track the process history of the data processings of an XCMSnExp object. This is in contrast to e.g. the CentWaveParam object that is passed to the actual processing method.

Usage

```
GenericParam(fun = character(), args = list())

## S4 method for signature 'GenericParam'
show(object)
```

Arguments

fun	character representing the name of the function.
args	list (ideally named) with the arguments to the function.
object	GenericParam object.

Value

The GenericParam function returns a GenericParam object.

Slots

fun character specifying the function name.

args list (ideally named) with the arguments to the function.

.__classVersion__ the version of the class.

Author(s)

Johannes Rainer

See Also

processHistory for how to access the process history of an XCMSnExp object.

Examples

```
prm <- GenericParam(fun = "mean")

prm <- GenericParam(fun = "mean", args = list(na.rm = TRUE))
```

getEIC-methods *Get extracted ion chromatograms for specified m/z ranges*

Description

Generate multiple extracted ion chromatograms for m/z values of interest. For xcmsSet objects, reread original raw data and apply precomputed retention time correction, if applicable.

Note that this method will *always* return profile, not raw data (with profile data being the binned data along M/Z). See details for further information.

Arguments

object	the xcmsRaw or xcmsSet object
mzrange	Either a two column matrix with minimum or maximum m/z or a matrix of any dimensions containing columns mzmin and mzmax. If not specified, the method for xcmsRaw returns the base peak chromatogram (BPC, i.e. the most intense signal for each RT across all m/z). For xcmsSet objects the group data will be used if mzrange is not provided.
rtrange	A two column matrix the same size as mzrange with minimum and maximum retention times between which to return EIC data points. If not specified, the method returns the chromatogram for the full RT range. For xcmsSet objects, it may also be a single number specifying the time window around the peak to return EIC data points
step	step (bin) size to use for profile generation. Note that a value of step = 0 is not supported.
groupidx	either character vector with names or integer vector with indicies of peak groups for which to get EICs
sampleidx	either character vector with names or integer vector with indicies of samples for which to get EICs
rt	"corrected" for using corrected retention times, or "raw" for using raw retention times

Details

In contrast to the rawEIC method, that extracts the actual raw values, this method extracts them from the object's profile matrix (or if the provided step argument does not match the profStep of the object the profile matrix is calculated on the fly and the values returned).

Value

For xcmsSet and xcmsRaw objects, an xcmsEIC object.

Methods

object = "xcmsRaw" `getEIC(object, mzrange, rtrange = NULL, step = 0.1)`

object = "xcmsSet" `getEIC(object, mzrange, rtrange = 200, groupidx, sampleidx = sampname`

See Also

xcmsRaw-class, xcmsSet-class, xcmsEIC-class, rawEIC

`getPeaks-methods` *Get peak intensities for specified regions*

Description

Integrate extracted ion chromatograms in pre-defined defined regions. Return output similar to `findPeaks`.

Arguments

`object`	the `xcmsSet` object
`peakrange`	matrix or data frame with 4 columns: `mzmin`, `mzmax`, `rtmin`, `rtmax` (they must be in that order or named)
`step`	step size to use for profile generation

Value

A matrix with columns:

`i`	rank of peak identified in merged EIC (<= `max`), always `NA`
`mz`	weighted (by intensity) mean of peak m/z across scans
`mzmin`	m/z of minimum step
`mzmax`	m/z of maximum step
`ret`	retention time of peak midpoint
`retmin`	leading edge of peak retention time
`retmax`	trailing edge of peak retention time
`into`	integrated area of original (raw) peak
`intf`	integrated area of filtered peak, always `NA`
`maxo`	maximum intensity of original (raw) peak
`maxf`	maximum intensity of filtered peak, always `NA`

Methods

object = "xcmsRaw" `getPeaks(object, peakrange, step = 0.1)`

See Also

`xcmsRaw-class`

getScan-methods *Get m/z and intensity values for a single mass scan*

Description

Return the data from a single mass scan using the numeric index of the scan as a reference.

Arguments

object	the xcmsRaw object
scan	integer index of scan. if negative, the index numbered from the end
mzrange	limit data points returned to those between in the range, range(mzrange)

Value

A matrix with two columns:

mz	m/z values
intensity	intensity values

Methods

object = "xcmsRaw" getScan(object, scan, mzrange = numeric()) getMsnScan(object, scan, mzrange = n

See Also

xcmsRaw-class, getSpec

getSpec-methods *Get average m/z and intensity values for multiple mass scans*

Description

Return full-resolution averaged data from multiple mass scans.

Arguments

object	the xcmsRaw object
...	arguments passed to profRange used to sepecify the spectral segments of interest for averaging

Details

Based on the mass points from the spectra selected, a master unique list of masses is generated. Every spectra is interpolated at those masses and then averaged.

Value

A matrix with two columns:

mz	m/z values
intensity	intensity values

Methods

object = "xcmsRaw" `getSpec(object, ...)`

See Also

xcmsRaw-class, profRange, getScan

`getXcmsRaw-methods` *Load the raw data for one or more files in the xcmsSet*

Description

Reads the raw data applies evential retention time corrections and waters Lock mass correction and returns it as an xcmsRaw object (or list of xcmsRaw objects) for one or more files of the xcmsSet object.

Arguments

object	the xcmsSet object
sampleidx	The index of the sample for which the raw data should be returned. Can be a single number or a numeric vector with the indices. Alternatively, the file name can be specified.
profmethod	The profile method.
profstep	The profile step.
rt	Whether corrected or raw retention times should be returned.
...	Additional arguments submitted to the xcmsRaw function.

Value

A single xcmsRaw object or a list of xcmsRaw objects.

Methods

object = "xcmsSet" `getXcmsRaw(object, sampleidx=1, profmethod=profinfo(object)$method, profstep=`
`)`

Author(s)

Johannes Rainer, <johannes.rainer@eurac.edu>

See Also

xcmsRaw-class,

group-methods *Group peaks from different samples together*

Description

A number of grouping (or alignment) methods exist in XCMS. group is the generic method.

Arguments

object	xcmsSet-class object
method	Method to use for grouping. See details.
...	Optional arguments to be passed along

Details

Different algorithms can be used by specifying them with the method argument. For example to use the density-based approach described by Smith et al (2006) one would use: group(object, method="density"). This is also the default.

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

A character vector of *nicknames* for the algorithms available is returned by getOption("BioC")$xcms$group.methods. If the nickname of a method is called "mzClust", the help page for that specific method can be accessed with ?group.mzClust.

Value

An xcmsSet object with peak group assignments and statistics.

Methods

object = "xcmsSet" group(object, ...)

See Also

group.density group.mzClust group.nearest xcmsSet-class,

group.density *Group peaks from different samples together*

Description

Group peaks together across samples using overlapping m/z bins and calculation of smoothed peak distributions in chromatographic time.

Arguments

object	the xcmsSet object
minfrac	minimum fraction of samples necessary in at least one of the sample groups for it to be a valid group
minsamp	minimum number of samples necessary in at least one of the sample groups for it to be a valid group
bw	bandwidth (standard deviation or half width at half maximum) of gaussian smoothing kernel to apply to the peak density chromatogram
mzwid	width of overlapping m/z slices to use for creating peak density chromatograms and grouping peaks across samples
max	maximum number of groups to identify in a single m/z slice
sleep	seconds to pause between plotting successive steps of the peak grouping algorithm. peaks are plotted as points showing relative intensity. identified groups are flanked by dotted vertical lines.

Value

An xcmsSet object with peak group assignments and statistics.

Methods

object = "xcmsSet" `group(object, bw = 30, minfrac = 0.5, minsamp = 1, mzwid = 0.25, max = 50,`

See Also

do_groupChromPeaks_density for the core API function performing the analysis. xcmsSet-class, density

---

group.mzClust *Group Peaks via High Resolution Alignment*

Description

Runs high resolution alignment on single spectra samples stored in a given xcmsSet.

Arguments

object	a xcmsSet with peaks
mzppm	the relative error used for clustering/grouping in ppm (parts per million)
mzabs	the absolute error used for clustering/grouping
minsamp	set the minimum number of samples in one bin
minfrac	set the minimum fraction of each class in one bin

Value

Returns a xcmsSet with slots groups and groupindex set.

Methods

object = "xcmsSet" `group(object, method="mzClust", mzppm = 20, mzabs = 0, minsamp = 1, minfrac=`

References

Saira A. Kazmi, Samiran Ghosh, Dong-Guk Shin, Dennis W. Hill and David F. Grant
Alignment of high resolution mass spectra: development of a heuristic approach for metabolomics.
Metabolomics, Vol. 2, No. 2, 75-83 (2006)

See Also

xcmsSet-class,

Examples

```
## Not run:
library(msdata)
mzdatapath <- system.file("fticr", package = "msdata")
mzdatafiles <- list.files(mzdatapath, recursive = TRUE, full.names = TRUE)

xs <- xcmsSet(method="MSW", files=mzdatafiles, scales=c(1,7), SNR.method='data.mean' , winSize.noise=500,
               peakThr=80000,  amp.Th=0.005)

xsg <- group(xs, method="mzClust")

## End(Not run)
```

---

group.nearest *Group peaks from different samples together*

Description

Group peaks together across samples by creating a master peak list and assigning corresponding peaks from all samples. It is inspired by the alignment algorithm of mzMine. For further details check http://mzmine.sourceforge.net/ and

Katajamaa M, Miettinen J, Oresic M: MZmine: Toolbox for processing and visualization of mass spectrometry based molecular profile data. Bioinformatics (Oxford, England) 2006, 22:634?636.

Currently, there is no equivalent to `minfrac` or `minsamp`.

Arguments

`object`	the `xcmsSet` object
`mzVsRTbalance`	Multiplicator for mz value before calculating the (euclidean) distance between two peaks.
`mzCheck`	Maximum tolerated distance for mz.
`rtCheck`	Maximum tolerated distance for RT.
`kNN`	Number of nearest Neighbours to check

Value

An xcmsSet object with peak group assignments and statistics.

Methods

object = "xcmsSet" `group(object, mzVsRTbalance=10, mzCheck=0.2, rtCheck=15, kNN=10)`

See Also

xcmsSet-class, group.density and group.mzClust

Examples

```
## Not run: library(xcms)
library(faahKO) ## These files do not have this problem to correct for but just for an example
cdfpath <- system.file("cdf", package = "faahKO")
cdffiles <- list.files(cdfpath, recursive = TRUE, full.names = TRUE)

xset<-xcmsSet(cdffiles)

gxset<-group(xset, method="nearest")
## this is the same as
# gxset<-group.nearest(xset)
nrow(gxset@groups) == 1096 ## the number of features before minFrac

post.minFrac<-function(object, minFrac=0.5){
ix.minFrac<-sapply(1:length(unique(sampclass(object))), function(x, object, mf){
meta<-groups(object)
minFrac.idx<-numeric(length=nrow(meta))
idx<-which(meta[,levels(sampclass(object))[x]] >= mf*length(which(levels(sampclass(object))[x] == sampclass
minFrac.idx[idx]<-1
return(minFrac.idx)
}, object, minFrac)
ix.minFrac<-as.logical(apply(ix.minFrac, 1, sum))
ix<-which(ix.minFrac == TRUE)
return(ix)
}

## using the above function we can get a post processing minFrac
idx<-post.minFrac(gxset)

gxset.post<-gxset ## copy the xcmsSet object
gxset.post@groupidx<-gxset@groupidx[idx]
gxset.post@groups<-gxset@groups[idx,]

nrow(gxset.post@groups) == 465 ## this is the number of features after minFrac

## End(Not run)
```

groupChromPeaks *Correspondence: Chromatographic peak grouping methods.*

Description

The groupChromPeaks method(s) perform the correspondence, i.e. the grouping of chromatographic peaks within and between samples. These methods are part of the modernized xcms user interface. The resulting peak groups are referred to as (mz-rt) features and can be accessed *via* the featureDefinitions method on the result object.

The implemented peak grouping methods are:

density peak grouping based on time dimension peak densities. See groupChromPeaks-density for more details.

mzClust high resolution peak grouping for single spectra (direct infusion) MS data. See groupChromPeaks-mzClust for more details.

nearest chromatographic peak grouping based on their proximity in the mz-rt space. See groupChromPeaks-nearest for more details.

Author(s)

Johannes Rainer

See Also

group for the *old* peak grouping methods. featureDefinitions and featureValues,XCMSnExp-method for methods to access peak grouping results.

Other peak grouping methods: groupChromPeaks-density, groupChromPeaks-mzClust, groupChromPeaks-nearest

groupChromPeaks-density *Peak grouping based on time dimension peak densities*

Description

This method performs performs correspondence (chromatographic peak grouping) based on the density (distribution) of identified peaks along the retention time axis within slices of overlapping mz ranges. All peaks (from the same or from different samples) being close on the retention time axis are grouped into a feature (*peak group*).

The PeakDensityParam class allows to specify all settings for the peak grouping based on peak densities along the time dimension. Instances should be created with the PeakDensityParam constructor.

sampleGroups,sampleGroups<-: getter and setter for the sampleGroups slot of the object. Its length should match the number of samples in the experiment and it should not contain NAs.

bw,bw<-: getter and setter for the bw slot of the object.

minFraction,minFraction<-: getter and setter for the minFraction slot of the object.

minSamples,minSamples<-: getter and setter for the minSamples slot of the object.

binSize,binSize<-: getter and setter for the binSize slot of the object.

maxFeatures,maxFeatures<-: getter and setter for the maxFeatures slot of the object.

groupChromPeaks,XCMSnExp,PeakDensityParam: performs correspondence (peak grouping within and across samples) within in mz dimension overlapping slices of MS data based on the density distribution of the identified chromatographic peaks in the slice along the time axis.

Usage

```
PeakDensityParam(sampleGroups = numeric(), bw = 30, minFraction = 0.5,
  minSamples = 1, binSize = 0.25, maxFeatures = 50)

## S4 method for signature 'PeakDensityParam'
show(object)

## S4 method for signature 'PeakDensityParam'
sampleGroups(object)

## S4 replacement method for signature 'PeakDensityParam'
sampleGroups(object) <- value

## S4 method for signature 'PeakDensityParam'
bw(object)

## S4 replacement method for signature 'PeakDensityParam'
bw(object) <- value

## S4 method for signature 'PeakDensityParam'
minFraction(object)

## S4 replacement method for signature 'PeakDensityParam'
minFraction(object) <- value

## S4 method for signature 'PeakDensityParam'
minSamples(object)

## S4 replacement method for signature 'PeakDensityParam'
minSamples(object) <- value

## S4 method for signature 'PeakDensityParam'
binSize(object)

## S4 replacement method for signature 'PeakDensityParam'
binSize(object) <- value

## S4 method for signature 'PeakDensityParam'
maxFeatures(object)

## S4 replacement method for signature 'PeakDensityParam'
maxFeatures(object) <- value

## S4 method for signature 'XCMSnExp,PeakDensityParam'
groupChromPeaks(object, param)
```

Arguments

sampleGroups	A vector of the same length than samples defining the sample group assignments (i.e. which samples belong to which sample group). This parameter is mandatory for the PeakDensityParam and has to be provided also if there is no sample grouping in the experiment (in which case all samples should be assigned to the same group).
bw	numeric(1) defining the bandwidth (standard deviation ot the smoothing kernel) to be used. This argument is passed to the density method.
minFraction	numeric(1) defining the minimum fraction of samples in at least one sample group in which the peaks have to be present to be considered as a peak group (feature).
minSamples	numeric(1) with the minimum number of samples in at least one sample group in which the peaks have to be detected to be considered a peak group (feature).
binSize	numeric(1) defining the size of the overlapping slices in mz dimension.
maxFeatures	numeric(1) with the maximum number of peak groups to be identified in a single mz slice.
object	For groupChromPeaks: an XCMSnExp object containing the results from a previous peak detection analysis (see findChromPeaks). For all other methods: a PeakDensityParam object.
value	The value for the slot.
param	A PeakDensityParam object containing all settings for the peak grouping algorithm.

Value

The PeakDensityParam function returns a PeakDensityParam class instance with all of the settings specified for chromatographic peak alignment based on peak densities. Note that argument 'sampleGroups' is mandatory and should represent either the sample grouping in the experiment. It's length has to match the number of sample in the experiments.

For groupChromPeaks: a XCMSnExp object with the results of the correspondence analysis. The definition of the resulting mz-rt features can be accessed with the featureDefinitions method.

Slots

.__classVersion__,sampleGroups,bw,minFraction,minSamples,binSize,maxFeatures See corresponding parameter above. .__classVersion__ stores the version from the class. Slots values should exclusively be accessed *via* the corresponding getter and setter methods listed above.

Note

These methods and classes are part of the updated and modernized xcms user interface which will eventually replace the group methods. All of the settings to the algorithm can be passed with a PeakDensityParam object.

Calling groupChromPeaks on an XCMSnExp object will cause all eventually present previous correspondence results to be dropped.

Author(s)

Colin Smith, Johannes Rainer

References

Colin A. Smith, Elizabeth J. Want, Grace O'Maille, Ruben Abagyan and Gary Siuzdak. "XCMS: Processing Mass Spectrometry Data for Metabolite Profiling Using Nonlinear Peak Alignment, Matching, and Identification" *Anal. Chem.* 2006, 78:779-787.

See Also

The do_groupChromPeaks_density core API function and group.density for the old user interface.

plotChromPeakDensity to plot peak densities and evaluate different algorithm settings. featureDefinitions and featureValues,XCMSnExp-method for methods to access the features (i.e. the peak grouping results).

XCMSnExp for the object containing the results of the correspondence.

Other peak grouping methods: groupChromPeaks-mzClust, groupChromPeaks-nearest, groupChromPeaks

Examples

```
## Create a PeakDensityParam object
p <- PeakDensityParam(binSize = 0.05, sampleGroups = c(1, 1, 2, 2))
## Change hte minSamples slot
minSamples(p) <- 3
p

##############################
## Chromatographic peak detection and grouping.
##
## Below we perform first a peak detection (using the matchedFilter
## method) on some of the test files from the faahKO package followed by
## a peak grouping using the density method.
library(faahKO)
library(MSnbase)
fls <- dir(system.file("cdf/KO", package = "faahKO"), recursive = TRUE,
           full.names = TRUE)

## Reading 2 of the KO samples
raw_data <- readMSData(fls[1:2], mode = "onDisk")

## Perform the chromatographic peak detection using the matchedFilter method.
mfp <- MatchedFilterParam(snthresh = 20, binSize = 1)
res <- findChromPeaks(raw_data, param = mfp)

head(chromPeaks(res))
## The number of peaks identified per sample:
table(chromPeaks(res)[, "sample"])

## Performing the chromatographic peak grouping. Assigning all samples to
## the same sample group.
fdp <- PeakDensityParam(sampleGroups = rep(1, length(fileNames(res))))
res <- groupChromPeaks(res, fdp)

## The definition of the features (peak groups):
featureDefinitions(res)

## Using the featureValues method to extract a matrix with the
```

```
## intensities of the features per sample.
head(featureValues(res, value = "into"))

## The process history:
processHistory(res)
```

---

groupChromPeaks-mzClust

High resolution peak grouping for single spectra samples

Description

This method performs high resolution correspondence for single spectra samples.

The MzClustParam class allows to specify all settings for the peak grouping based on the *mzClust* algorithm. Instances should be created with the MzClustParam constructor.

sampleGroups,sampleGroups<-: getter and setter for the sampleGroups slot of the object.

ppm,ppm<-: getter and setter for the ppm slot of the object.

absMz,absMz<-: getter and setter for the absMz slot of the object.

minFraction,minFraction<-: getter and setter for the minFraction slot of the object.

minSamples,minSamples<-: getter and setter for the minSamples slot of the object.

groupChromPeaks,XCMSnExp,MzClustParam: performs high resolution peak grouping for single spectrum metabolomics data.

Usage

```
MzClustParam(sampleGroups = numeric(), ppm = 20, absMz = 0,
  minFraction = 0.5, minSamples = 1)

## S4 method for signature 'MzClustParam'
show(object)

## S4 method for signature 'MzClustParam'
sampleGroups(object)

## S4 replacement method for signature 'MzClustParam'
sampleGroups(object) <- value

## S4 method for signature 'MzClustParam'
ppm(object)

## S4 replacement method for signature 'MzClustParam'
ppm(object) <- value

## S4 method for signature 'MzClustParam'
absMz(object)

## S4 replacement method for signature 'MzClustParam'
absMz(object) <- value
```

```
## S4 method for signature 'MzClustParam'
minFraction(object)

## S4 replacement method for signature 'MzClustParam'
minFraction(object) <- value

## S4 method for signature 'MzClustParam'
minSamples(object)

## S4 replacement method for signature 'MzClustParam'
minSamples(object) <- value

## S4 method for signature 'XCMSnExp,MzClustParam'
groupChromPeaks(object, param)
```

Arguments

sampleGroups	A vector of the same length than samples defining the sample group assignments (i.e. which samples belong to which sample group). This parameter is mandatory for the PeakDensityParam and has to be provided also if there is no sample grouping in the experiment (in which case all samples should be assigned to the same group).
ppm	numeric(1) representing the relative mz error for the clustering/grouping (in parts per million).
absMz	numeric(1) representing the absolute mz error for the clustering.
minFraction	numeric(1) defining the minimum fraction of samples in at least one sample group in which the peaks have to be present to be considered as a peak group (feature).
minSamples	numeric(1) with the minimum number of samples in at least one sample group in which the peaks have to be detected to be considered a peak group (feature).
object	For groupChromPeaks: an XCMSnExp object containing the results from a previous chromatographic peak detection analysis (see findChromPeaks). For all other methods: a MzClustParam object.
value	The value for the slot.
param	A MzClustParam object containing all settings for the peak grouping algorithm.

Value

The MzClustParam function returns a MzClustParam class instance with all of the settings specified for high resolution single spectra peak alignment.

For groupChromPeaks: a XCMSnExp object with the results of the peak grouping step (i.e. the features). These can be accessed with the featureDefinitions method.

Slots

.__classVersion__,sampleGroups,ppm,absMz,minFraction,minSamples See corresponding parameter above. .__classVersion__ stores the version from the class. Slots values should exclusively be accessed *via* the corresponding getter and setter methods listed above.

Note

These methods and classes are part of the updated and modernized xcms user interface which will eventually replace the group methods. All of the settings to the algorithm can be passed with a MzClustParam object.

Calling groupChromPeaks on an XCMSnExp object will cause all eventually present previous correspondence results to be dropped.

References

Saira A. Kazmi, Samiran Ghosh, Dong-Guk Shin, Dennis W. Hill and David F. Grant
Alignment of high resolution mass spectra: development of a heuristic approach for metabolomics.
Metabolomics, Vol. 2, No. 2, 75-83 (2006)

See Also

The do_groupPeaks_mzClust core API function and group.mzClust for the old user interface. featureDefinitions and featureValues,XCMSnExp-method for methods to access peak grouping results (i.e. the features).

XCMSnExp for the object containing the results of the peak grouping.

Other peak grouping methods: groupChromPeaks-density, groupChromPeaks-nearest, groupChromPeaks

Examples

```
## Loading a small subset of direct injection, single spectrum files
library(msdata)
fticrf <- list.files(system.file("fticr", package = "msdata"),
                     recursive = TRUE, full.names = TRUE)
fticr <- readMSData(fticrf[1:2], msLevel. = 1, mode = "onDisk")

## Perform the MSW peak detection on these:
p <- MSWParam(scales = c(1, 7), peakThr = 80000, ampTh = 0.005,
              SNR.method = "data.mean", winSize.noise = 500)
fticr <- findChromPeaks(fticr, param = p)

head(chromPeaks(fticr))

## Now create the MzClustParam parameter object: we're assuming here that
## both samples are from the same sample group.
p <- MzClustParam(sampleGroups = c(1, 1))

fticr <- groupChromPeaks(fticr, param = p)

## Get the definition of the features.
featureDefinitions(fticr)
```

---

groupChromPeaks-nearest *Peak grouping based on proximity in the mz-rt space*

Description

This method is inspired by the grouping algorithm of mzMine [Katajamaa 2006] and performs correspondence based on proximity of peaks in the space spanned by retention time and mz values. The method creates first a *master peak list* consisting of all chromatographic peaks from the sample in which most peaks were identified, and starting from that, calculates distances to peaks from the sample with the next most number of peaks. If peaks are closer than the defined threshold they are grouped together.

The `NearestPeaksParam` class allows to specify all settings for the peak grouping based on the *nearest* algorithm. Instances should be created with the `NearestPeaksParam` constructor.

`sampleGroups,sampleGroups<-`: getter and setter for the `sampleGroups` slot of the object.

`mzVsRtBalance,mzVsRtBalance<-`: getter and setter for the `mzVsRtBalance` slot of the object.

`absMz,absMz<-`: getter and setter for the `absMz` slot of the object.

`absRt,absRt<-`: getter and setter for the `absRt` slot of the object.

`kNN,kNN<-`: getter and setter for the `kNN` slot of the object.

`groupChromPeaks,XCMSnExp,NearestPeaksParam`: performs peak grouping based on the proximity between chromatographic peaks from different samples in the mz-rt range.

Usage

```
NearestPeaksParam(sampleGroups = numeric(), mzVsRtBalance = 10,
  absMz = 0.2, absRt = 15, kNN = 10)

## S4 method for signature 'NearestPeaksParam'
show(object)

## S4 method for signature 'NearestPeaksParam'
sampleGroups(object)

## S4 replacement method for signature 'NearestPeaksParam'
sampleGroups(object) <- value

## S4 method for signature 'NearestPeaksParam'
mzVsRtBalance(object)

## S4 replacement method for signature 'NearestPeaksParam'
mzVsRtBalance(object) <- value

## S4 method for signature 'NearestPeaksParam'
absMz(object)

## S4 replacement method for signature 'NearestPeaksParam'
absMz(object) <- value

## S4 method for signature 'NearestPeaksParam'
absRt(object)

## S4 replacement method for signature 'NearestPeaksParam'
absRt(object) <- value

## S4 method for signature 'NearestPeaksParam'
```

```
kNN(object)

## S4 replacement method for signature 'NearestPeaksParam'
kNN(object) <- value

## S4 method for signature 'XCMSnExp,NearestPeaksParam'
groupChromPeaks(object, param)
```

Arguments

sampleGroups	A vector of the same length than samples defining the sample group assignments (i.e. which samples belong to which sample group). This parameter is mandatory for the PeakDensityParam and has to be provided also if there is no sample grouping in the experiment (in which case all samples should be assigned to the same group).
mzVsRtBalance	numeric(1) representing the factor by which mz values are multiplied before calculating the (euclician) distance between two peaks.
absMz	numeric(1) maximum tolerated distance for mz values.
absRt	numeric(1) maximum tolerated distance for rt values.
kNN	numeric(1) representing the number of nearest neighbors to check.
object	For groupChromPeaks: an XCMSnExp object containing the results from a previous chromatographic peak detection analysis (see findChromPeaks). For all other methods: a NearestPeaksParam object.
value	The value for the slot.
param	A NearestPeaksParam object containing all settings for the peak grouping algorithm.

Value

The NearestPeaksParam function returns a NearestPeaksParam class instance with all of the settings specified for peak alignment based on peak proximity.

For groupChromPeaks: a XCMSnExp object with the results of the peak grouping/correspondence step (i.e. the mz-rt features). These can be accessed with the featureDefinitions method.

Slots

.__classVersion__,sampleGroups,mzVsRtBalance,absMz,absRt,kNN See corresponding parameter above. .__classVersion__ stores the version from the class. Slots values should exclusively be accessed *via* the corresponding getter and setter methods listed above.

Note

These methods and classes are part of the updated and modernized xcms user interface which will eventually replace the group methods. All of the settings to the algorithm can be passed with a NearestPeaksParam object.

Calling groupChromPeaks on an XCMSnExp object will cause all eventually present previous alignment results to be dropped.

References

Katajamaa M, Miettinen J, Oresic M: MZmine: Toolbox for processing and visualization of mass spectrometry based molecular profile data. *Bioinformatics* 2006, 22:634-636.

See Also

The do_groupChromPeaks_nearest core API function and group.nearest for the old user interface. featureDefinitions and featureValues,XCMSnExp-method for methods to access peak grouping results (i.e. the features).

XCMSnExp for the object containing the results of the peak grouping.

Other peak grouping methods: groupChromPeaks-density, groupChromPeaks-mzClust, groupChromPeaks

Examples

```
## Create a NearestPeaksParam object
p <- NearestPeaksParam(kNN = 3)
p

##############################
## Chromatographic peak detection and grouping.
##
## Below we perform first a chromatographic peak detection (using the
## matchedFilter method) on some of the test files from the faahKO package
## followed by a peaks grouping using the "nearest" method.
library(faahKO)
library(MSnbase)
fls <- dir(system.file("cdf/KO", package = "faahKO"), recursive = TRUE,
           full.names = TRUE)

## Reading 2 of the KO samples
raw_data <- readMSData(fls[1:2], mode = "onDisk")

## Perform the peak detection using the matchedFilter method.
mfp <- MatchedFilterParam(snthresh = 20, binSize = 1)
res <- findChromPeaks(raw_data, param = mfp)

head(chromPeaks(res))
## The number of peaks identified per sample:
table(chromPeaks(res)[, "sample"])

## Performing the peak grouping
p <- NearestPeaksParam()
res <- groupChromPeaks(res, param = p)

## The results from the peak grouping:
featureDefinitions(res)

## Using the featureValues method to extract a matrix with the intensities of
## the features per sample.
head(featureValues(res, value = "into"))

## The process history:
processHistory(res)
```

---

groupnames-methods *Generate unque names for peak groups*

Description

Allow linking of peak group data between classes using unique group names that remain the same as long as no re-grouping occurs.

Arguments

object	the xcmsSet or xcmsEIC object
mzdec	number of decimal places to use for m/z
rtdec	number of decimal places to use for retention time
template	a character vector with existing group names whose format should be emulated

Value

A character vector with unique names for each peak group in the object. The format is M[m/z]T[time in seconds].

Methods

object = "xcmsSet" `(object, mzdec = 0, rtdec = 0, template = NULL)`

object = "xcmsEIC" `(object)`

See Also

xcmsSet-class, xcmsEIC-class

---

groupval-methods *Extract a matrix of peak values for each group*

Description

Generate a matrix of peak values with rows for every group and columns for every sample. The value included in the matrix can be any of the columns from the xcmsSet peaks slot matrix. Collisions where more than one peak from a single sample are in the same group get resolved with one of several user-selectable methods.

Arguments

object	the xcmsSet object
method	conflict resolution method, "medret" to use the peak closest to the median retention time or "maxint" to use the peak with the highest intensity
value	name of peak column to enter into returned matrix, or "index" for index to the corresponding row in the peaks slot matrix
intensity	if method == "maxint", name of peak column to use for intensity

Value

A matrix with with rows for every group and columns for every sample. Missing peaks have NA values.

Methods

object = "xcmsSet" `groupval(object, method = c("medret", "maxint"), value = "index", i`

See Also

xcmsSet-class

---

highlightChromPeaks *Add definition of chromatographic peaks to an extracted chromatogram plot*

Description

The highlightChromPeaks function adds chromatographic peak definitions to an existing plot, such as one created by the plot method on a Chromatogram or Chromatograms object.

Usage

```
highlightChromPeaks(x, rt, mz, border = rep("00000040", length(fileNames(x))),
  lwd = 1, col = NA, type = c("rect", "point"), ...)
```

Arguments

x	For highlightChromPeaks: XCMSnExp object with the detected peaks.
rt	For highlightChromPeaks: numeric(2) with the retention time range from which peaks should be extracted and plotted.
mz	numeric(2) with the mz range from which the peaks should be extracted and plotted.
border	colors to be used to color the border of the rectangles. Has to be equal to the number of samples in x.
lwd	numeric(1) defining the width of the line/border.
col	For highlightChromPeaks: color to be used to fill the rectangle.
type	the plotting type. See plot for more details. For highlightChromPeaks: character(1) defining how the peak should be highlighted: type = "rect" draws a rectangle representing the peak definition, type = "point" indicates a chromatographic peak with a single point at the position of the peak's "rt" and "maxo".
...	additional parameters to the matplot or plot function.

Author(s)

Johannes Rainer

Examples

```
## Read some files from the faahKO package.
library(xcms)
library(faahKO)
faahko_3_files <- c(system.file('cdf/KO/ko16.CDF', package = "faahKO"),
                    system.file('cdf/KO/ko18.CDF', package = "faahKO"))

od <- readMSData(faahko_3_files, mode = "onDisk")

## Peak detection using the 'matchedFilter' method. Note that we are using a
## larger binSize to reduce the runtime of the example.
xod <- findChromPeaks(od, param = MatchedFilterParam(binSize = 0.3, snthresh = 20))

## Extract the ion chromatogram for one chromatographic peak in the data.
chrs <- chromatogram(xod, rt = c(2700, 2900), mz = 335)

plot(chrs)

## Extract chromatographic peaks for the mz/rt range (if any).
chromPeaks(xod, rt = c(2700, 2900), mz = 335)

## Highlight the chromatographic peaks in the area
highlightChromPeaks(xod, rt = c(2700, 2900), mz = 335)
```

`image-methods` *Plot log intensity image of a xcmsRaw object*

Description

Create log intensity false-color image of a xcmsRaw object plotted with m/z and retention time axes

Arguments

`x`	xcmsRaw object
`col`	vector of colors to use for for the image
`...`	arguments for `profRange`

Methods

x = "xcmsRaw" `image(x, col = rainbow(256), ...)`

Author(s)

Colin A. Smith, <csmith@scripps.edu>

See Also

xcmsRaw-class

`imputeLinInterpol` *Impute values for empty elements in a vector using linear interpolation*

Description

This function provides missing value imputation based on linear interpolation and resembles some of the functionality of the `profBinLin` and `profBinLinBase` functions deprecated from version 1.51 on.

Usage

```
imputeLinInterpol(x, baseValue, method = "lin", distance = 1L,
  noInterpolAtEnds = FALSE)
```

Arguments

`x`	A numeric vector with eventual missing (`NA`) values.
`baseValue`	The base value to which empty elements should be set. This is only considered for `method = "linbase"` and corresponds to the `profBinLinBase`'s `baselevel` argument.
`method`	One of `"none"`, `"lin"` or `"linbase"`.
`distance`	For `method = "linbase"`: number of non-empty neighboring element of an empty element that should be considered for linear interpolation. See details section for more information.
`noInterpolAtEnds`	For `method = "lin"`: Logical indicating whether linear interpolation should also be performed at the ends of the data vector (i.e. if missing values are present at the beginning or the end of the vector).

Details

Values for NAs in input vector `x` can be imputed using methods `"lin"` and `"linbase"`:

`impute = "lin"` uses simple linear imputation to derive a value for an empty element in input vector `x` from its neighboring non-empty elements. This method is equivalent to the linear interpolation in the `profBinLin` method. Whether interpolation is performed if missing values are present at the beginning and end of `x` can be set with argument `noInterpolAtEnds`. By default interpolation is also performed at the ends interpolating from `0` at the beginning and towards `0` at the end. For `noInterpolAtEnds = TRUE` no interpolation is performed at both ends replacing the missing values at the beginning and/or the end of `x` with `0`.

`impute = "linbase"` uses linear interpolation to impute values for empty elements within a user-definable proximity to non-empty elements and setting the element's value to the `baseValue` otherwise. The default for the `baseValue` is half of the smallest value in `x` (`NA`s being removed). Whether linear interpolation based imputation is performed for a missing value depends on the `distance` argument. Interpolation is only performed if one of the next `distance` closest neighbors to the current empty element has a value other than `NA`. No interpolation takes place for `distance = 0`, while `distance = 1` means that the value for an empty element is interpolated from directly adjacent non-empty elements while, if the next neighbors of the current empty element are also `NA`, it's vale is set to `baseValue`. This corresponds to the linear interpolation performed by the `profBinLinBase` method. For more details see examples below.

Value

A numeric vector with empty values imputed based on the selected method.

Author(s)

Johannes Rainer

Examples

```
#######
## Impute missing values by linearly interpolating from neighboring
## non-empty elements
x <- c(3, NA, 1, 2, NA, NA, 4, NA, NA, NA, 3, NA, NA, NA, NA, 2)
imputeLinInterpol(x, method = "lin")
## visualize the interpolation:
plot(x = 1:length(x), y = x)
points(x = 1:length(x), y = imputeLinInterpol(x, method = "lin"), type = "l", col = "grey")

## If the first or last elements are NA, interpolation is performed from 0
## to the first non-empty element.
x <- c(NA, 2, 1, 4, NA)
imputeLinInterpol(x, method = "lin")
## visualize the interpolation:
plot(x = 1:length(x), y = x)
points(x = 1:length(x), y = imputeLinInterpol(x, method = "lin"), type = "l", col = "grey")

## If noInterpolAtEnds is TRUE no interpolation is performed at both ends
imputeLinInterpol(x, method = "lin", noInterpolAtEnds = TRUE)

######
## method = "linbase"
## "linbase" performs imputation by interpolation for empty elements based on
## 'distance' adjacent non-empty elements, setting all remaining empty elements
## to the baseValue
x <- c(3, NA, 1, 2, NA, NA, 4, NA, NA, NA, 3, NA, NA, NA, NA, 2)
## Setting distance = 0 skips imputation by linear interpolation
imputeLinInterpol(x, method = "linbase", distance = 0)

## With distance = 1 for all empty elements next to a non-empty element the value
## is imputed by linear interpolation.
xInt <- imputeLinInterpol(x, method = "linbase", distance = 1L)
xInt

plot(x = 1:length(x), y = x, ylim = c(0, max(x, na.rm = TRUE)))
points(x = 1:length(x), y = xInt, type = "l", col = "grey")

## Setting distance = 2L would cause that for all empty elements for which the
## distance to the next non-empty element is <= 2 the value is imputed by
## linear interpolation:
xInt <- imputeLinInterpol(x, method = "linbase", distance = 2L)
xInt

plot(x = 1:length(x), y = x, ylim = c(0, max(x, na.rm = TRUE)))
points(x = 1:length(x), y = xInt, type = "l", col = "grey")
```

levelplot-methods *Plot log intensity image of a xcmsRaw object*

Description

Create an image of the raw (profile) data m/z against retention time, with the intensity color coded.

Arguments

x	xcmsRaw object.
log	Whether the intensity should be log transformed.
col.regions	The color ramp that should be used for encoding of the intensity.
rt	wheter the original (rt="raw") or the corrected (rt="corrected") retention times should be used.
...	Arguments for profRange.

Methods

x = "xcmsRaw" `levelplot(x, log=TRUE, col.regions=colorRampPalette(brewer.pal(9, "YlOrRd"))`

x = "xcmsSet" `levelplot(x, log=TRUE, col.regions=colorRampPalette(brewer.pal(9, "YlOrRd"))(`

Author(s)

Johannes Rainer, <johannes.rainer@eurac.edu>

See Also

xcmsRaw-class, xcmsSet-class

loadRaw-methods *Read binary data from a source*

Description

This function extracts the raw data which will be used an xcmsRaw object. Further processing of data is done in the xcmsRaw constructor.

Arguments

object	Specification of a data source (such as a file name or database query)

Details

The implementing methods decide how to gather the data.

Value

A list containing elements describing the data source. The `rt`, `scanindex`, `tic`, and `acquisitionNum` components each have one entry per scan. They are *parallel* in the sense that `rt[1]`, `scanindex[1]`, and `acquisitionNum[1]` all refer to the same scan. The list containst the following components:

`rt`	Numeric vector with acquisition time (in seconds) for each scan
`tic`	Numeric vector with Total Ion Count for each scan
`scanindex`	Integer vector with starting positions of each scan in the `mz` and `intensity` components. It is an exclusive offset, so `scanindex[i]` is the offset in `mz` and `intensity` *before* the beginning of scan `i`. This means that the `mz` (respectively `intensity`) values for scan `i` would be from `scanindex[i] + 1` to `scanindex[i + 1]`
`mz`	Concatenated vector of m/z values for all scans
`intensity`	Concatenated vector of intensity values for all scans

Methods

`signature(object = "xcmsSource")` Uses `loadRaw,xcmsSource-method` to extract raw data. Subclasses of `xcmsSource` can provide different ways of fetching data.

Author(s)

Daniel Hackney, <dan@haxney.org>

See Also

`xcmsRaw-class`, `xcmsSource`

`medianFilter` *Apply a median filter to a matrix*

Description

For each element in a matix, replace it with the median of the values around it.

Usage

```
medianFilter(x, mrad, nrad)
```

Arguments

`x`	numeric matrix to median filter
`mrad`	number of rows on either side of the value to use for median calculation
`nrad`	number of rows on either side of the value to use for median calculation

Value

A matrix whose values have been median filtered

Author(s)

Colin A. Smith, <csmith@scripps.edu>

Examples

```
mat <- matrix(1:25, nrow=5)
mat
medianFilter(mat, 1, 1)
```

---

msn2xcmsRaw *Copy MSn data in an xcmsRaw to the MS slots*

Description

The MS2 and MSn data is stored in separate slots, and can not directly be used by e.g. findPeaks(). `msn2xcmsRaw()` will copy the MSn spectra into the "normal" `xcmsRaw` slots.

Usage

```
msn2xcmsRaw(xmsn)
```

Arguments

`xmsn`	an object of class `xcmsRaw` that contains spectra read with includeMSn=TRUE

Details

The default gap value is determined from the 90th percentile of the pair-wise differences between adjacent mass values.

Value

An xcmsRaw object

Author(s)

Steffen Neumann <sneumann@ipb-halle.de>

See Also

xcmsRaw,

Examples

```
msnfile <- system.file("microtofq/MSMSpos20_6.mzML", package = "msdata")
xrmsn <- xcmsRaw(msnfile, includeMSn=TRUE)
xr <- msn2xcmsRaw(xrmsn)
p <- findPeaks(xr, method="centWave")
```

peakPlots-methods *Plot a grid of a large number of peaks*

Description

Plot extracted ion chromatograms for many peaks simultaneously, indicating peak integration start and end points with vertical grey lines.

Arguments

object	the xcmsRaw object
peaks	matrix with peak information as produced by findPeaks
figs	two-element vector describing the number of rows and the number of columns of peaks to plot, if missing then an approximately square grid that will fit the number of peaks supplied
width	width of chromatogram retention time to plot for each peak

Details

This function is intended to help graphically analyze the results of peak picking. It can help estimate the number of false positives and improper integration start and end points. Its output is very compact and tries to waste as little space as possible. Each plot is labeled with rounded m/z and retention time separated by a space.

Methods

```
signature(object = "xcmsSet") plotPeaks(object, peaks, figs, width = 200)
```

See Also

xcmsRaw-class, findPeaks, split.screen

peakTable-methods *Create report of aligned peak intensities*

Description

Create a report showing all aligned peaks.

Arguments

object	the xcmsSet object
filebase	base file name to save report, .tsv file and _eic will be appended to this name for the tabular report and EIC directory, respectively. if blank nothing will be saved
...	arguments passed down to groupval, which provides the actual intensities.

Details

This method handles creation of summary reports similar to `diffreport`. It returns a summary report that can optionally be written out to a tab-separated file.

If a base file name is provided, the report (see Value section) will be saved to a tab separated file.

Value

A data frame with the following columns:

`mz`	median m/z of peaks in the group
`mzmin`	minimum m/z of peaks in the group
`mzmax`	maximum m/z of peaks in the group
`rt`	median retention time of peaks in the group
`rtmin`	minimum retention time of peaks in the group
`rtmax`	maximum retention time of peaks in the group
`npeaks`	number of peaks assigned to the group
`Sample Classes`	number samples from each sample class represented in the group
`...`	one column for every sample class
`Sample Names`	integrated intensity value for every sample
`...`	one column for every sample

Methods

object = "xcmsSet" `peakTable(object, filebase = character(), ...)`

See Also

`xcmsSet-class`,

Examples

```
## Not run:
library(faahKO)
cdfpath <- system.file("cdf", package = "faahKO")
cdffiles <- list.files(cdfpath, recursive = TRUE, full.names = TRUE)
xs<-xcmsSet(cdf files)
xs<-group(xs)
peakTable(xs, filebase="peakList")

## End(Not run)
```

phenoDataFromPaths *Derive experimental design from file paths*

Description

The phenoDataFromPaths function builds a data.frame representing the experimental design from the folder structure in which the files of the experiment are located.

Usage

```
phenoDataFromPaths(paths)
```

Arguments

paths	character representing the file names (including the full path) of the experiment's files.

Note

This function is used by the *old* xcmsSet function to guess the experimental design (i.e. group assignment of the files) from the folders in which the files of the experiment can be found.

Examples

```
## List the files available in the faahKO package
base_dir <- system.file("cdf", package = "faahKO")
cdf_files <- list.files(base_dir, recursive = TRUE, full.names = TRUE)
```

plot.xcmsEIC *Plot extracted ion chromatograms from multiple files*

Description

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

Arguments

x	the xcmsEIC object
y	optional xcmsSet object with peak integration data
groupidx	either character vector with names or integer vector with indicies of peak groups for which to plot EICs
sampleidx	either character vector with names or integer vector with indicies of samples for which to plot EICs
rtrange	a two column matrix with minimum and maximum retention times between which to return EIC data points if it has the same number of rows as the number groups in the xcmsEIC object, then sampleidx is used to subset it. otherwise, it is repeated over the length of sampleidx it may also be a single number specifying the time window around the peak for which to plot EIC data

col	color to use for plotting extracted ion chromatograms. if missing and y is specified, colors are taken from unclass(sampclass(y)) and the default palette if it is the same length as the number groups in the xcmsEIC object, then sampleidx is used to subset it. otherwise, it is repeated over the length of sampleidx
legtext	text to use for legend. if NULL and y is specified, legend text is taken from the sample class information found in the xcmsSet
peakint	logical, plot integrated peak area with darkened lines (requires that y also be specified)
sleep	seconds to pause between plotting EICs
...	other graphical parameters

Value

A xcmsSet object.

Methods

x = "xcmsEIC" `plot.xcmsEIC(x, y, groupidx = groupnames(x), sampleidx = sampnames(x), rtrange = x@`

Author(s)

Colin A. Smith, <csmith@scripps.edu>

See Also

xcmsEIC-class, png, pdf, postscript,

---

plotAdjustedRtime *Visualization of alignment results*

Description

Plot the difference between the adjusted and the raw retention time (y-axis) for each file along the (adjusted or raw) retention time (x-axis). If alignment was performed using the adjustRtime-peakGroups method, also the features (peak groups) used for the alignment are shown.

Usage

```
plotAdjustedRtime(object, col = "#00000080", lty = 1, type = "l",
  adjustedRtime = TRUE, xlab = ifelse(adjustedRtime, yes =
  expression(rt[adj]), no = expression(rt[raw])), ylab = expression(rt[adj] -
  rt[raw]), peakGroupsCol = "#00000060", peakGroupsPch = 16,
  peakGroupsLty = 3, ...)
```

Arguments

object	A XCMSnExp object with the alignment results.
col	colors to be used for the lines corresponding to the individual samples.
lty	line type to be used for the lines of the individual samples.
type	plot type to be used. See help on the par function for supported values.
adjustedRtime	logical(1) whether adjusted or raw retention times should be shown on the x-axis.
xlab	the label for the x-axis.
ylab	the label for the y-axis.
peakGroupsCol	color to be used for the peak groups (only used if alignment was performed using the adjustRtime-peakGroups method.
peakGroupsPch	point character (pch) to be used for the peak groups (only used if alignment was performed using the adjustRtime-peakGroups method.
peakGroupsLty	line type (lty) to be used to connect points for each peak groups (only used if alignment was performed using the adjustRtime-peakGroups method.
...	Additional arguments to be passed down to the plot function.

Author(s)

Johannes Rainer

See Also

adjustRtime for all retention time correction/ alignment methods.

Examples

```
## Below we perform first a peak detection (using the matchedFilter
## method) on some of the test files from the faahKO package followed by
## a peak grouping and retention time adjustment using the "peak groups"
## method
library(faahKO)
library(xcms)
fls <- dir(system.file("cdf/KO", package = "faahKO"), recursive = TRUE,
           full.names = TRUE)

## Reading 2 of the KO samples
raw_data <- readMSData(fls[1:2], mode = "onDisk")

## Perform the peak detection using the matchedFilter method.
mfp <- MatchedFilterParam(snthresh = 20, binSize = 1)
res <- findChromPeaks(raw_data, param = mfp)

## Performing the peak grouping using the "peak density" method.
p <- PeakDensityParam(sampleGroups = c(1, 1))
res <- groupChromPeaks(res, param = p)

## Perform the retention time adjustment using peak groups found in both
## files.
fgp <- PeakGroupsParam(minFraction = 1)
res <- adjustRtime(res, param = fgp)
```

```
## Visualize the impact of the alignment. We show both versions of the plot,
## with the raw retention times on the x-axis (top) and with the adjusted
## retention times (bottom).
par(mfrow = c(2, 1))
plotAdjustedRtime(res, adjusted = FALSE)
grid()
plotAdjustedRtime(res)
grid()
```

---

plotChrom-methods *Plot extracted ion chromatograms from the profile matrix*

Description

Uses the pre-generated profile mode matrix to plot averaged or base peak extracted ion chromatograms over a specified mass range.

Arguments

object	the xcmsRaw object
base	logical, plot a base-peak chromatogram
ident	logical, use mouse to identify and label peaks
fitgauss	logical, fit a gaussian to the largest peak
vline	numeric vector with locations of vertical lines
...	arguments passed to profRange

Value

If ident == TRUE, an integer vector with the indecies of the points that were identified. If fitgauss == TRUE, a nls model with the fitted gaussian. Otherwise a two-column matrix with the plotted points.

Methods

object = "xcmsRaw" plotChrom(object, base = FALSE, ident = FALSE, fitgauss = FALSE, v

See Also

xcmsRaw-class

plotChromPeakDensity *Plot chromatographic peak density along the retention time axis*

Description

Plot the density of chromatographic peaks along the retention time axis and indicate which peaks would be (or were) grouped into the same feature based using the *peak density* correspondence method. Settings for the *peak density* method can be passed with an PeakDensityParam object to parameter `param`. If the `object` contains correspondence results and the correspondence was performed with the *peak groups* method, the results from that correspondence can be visualized setting `simulate = FALSE`.

Usage

```
plotChromPeakDensity(object, mz, rt, param, simulate = TRUE,
  col = "#00000080", xlab = "retention time", ylab = "sample",
  xlim = range(rt), main = NULL, ...)
```

Arguments

`object`	A XCMSnExp object with identified chromatographic peaks.
`mz`	`numeric(2)` defining an mz range for which the peak density should be plotted.
`rt`	`numeric(2)` defining an optional rt range for which the peak density should be plotted. Defaults to the absolute retention time range of `object`.
`param`	PeakDensityParam from which parameters for the *peak density* correspondence algorithm can be extracted. If not provided and if `object` contains feature definitions with the correspondence/ peak grouping being performed by the *peak density* method, the corresponding parameter class stored in `object` is used.
`simulate`	`logical(1)` defining whether correspondence should be simulated within the specified m/z / rt region or (with `simulate = FALSE`) whether the results from an already performed correspondence should be shown.
`col`	Color to be used for the individual samples. Length has to be 1 or equal to the number of samples in `object`.
`xlab`	`character(1)` with the label for the x-axis.
`ylab`	`character(1)` with the label for the y-axis.
`xlim`	`numeric(2)` representing the limits for the x-axis. Defaults to the range of the `rt` parameter.
`main`	`character(1)` defining the title of the plot. By default (for `main = NULL`) the mz-range is used.
`...`	Additional parameters to be passed to the `plot` function. Data point specific parameters such as `bg` or `pch` have to be of length 1 or equal to the number of samples.

Details

The `plotChromPeakDensity` function allows to evaluate different settings for the *peak density* on an mz slice of interest (e.g. containing chromatographic peaks corresponding to a known metabolite). The plot shows the individual peaks that were detected within the specified `mz` slice at their retention time (x-axis) and sample in which they were detected (y-axis). The density function is plotted as a black line. Parameters for the `density` function are taken from the `param` object. Grey rectangles indicate which chromatographic peaks would be grouped into a feature by the `peak density` correspondence method. Parameters for the algorithm are also taken from `param`. See `groupChromPeaks-density()` for more information about the algorithm and its supported settings.

Value

The function is called for its side effect, i.e. to create a plot.

Author(s)

Johannes Rainer

See Also

`groupChromPeaks-density()` for details on the *peak density* correspondence method and supported settings.

Examples

```
## Below we perform first a peak detection (using the centWave
## method) on some of the test files from the faahKO package.
library(faahKO)
library(xcms)
fls <- dir(system.file("cdf/KO", package = "faahKO"), recursive = TRUE,
           full.names = TRUE)

## Reading 2 of the KO samples
raw_data <- readMSData(fls[1:2], mode = "onDisk")

## Perform the peak detection using the centWave method (settings are tuned
## to speed up example execution)
res <- findChromPeaks(raw_data, param = CentWaveParam(noise = 3000, snthresh = 40))

## Align the samples using obiwarp
res <- adjustRtime(res, param = ObiwarpParam())

## Plot the chromatographic peak density for a specific mz range to evaluate
## different peak density correspondence settings.
mzr <- c(305.05, 305.15)

plotChromPeakDensity(res, mz = mzr, pch = 16,
    param = PeakDensityParam(sampleGroups = rep(1, length(fileNames(res)))))

## Use a larger bandwidth
plotChromPeakDensity(res, mz = mzr, param = PeakDensityParam(bw = 60,
    sampleGroups = rep(1, length(fileNames(res)))), pch = 16)
## Neighboring peaks are now fused into one.
```

```
## Require the chromatographic peak to be present in all samples of a group
plotChromPeakDensity(res, mz = mzr, pch = 16,
    param = PeakDensityParam(minFraction = 1,
    sampleGroups = rep(1, length(fileNames(res)))))
```

---

plotChromPeaks *General visualizations of peak detection results*

Description

plotChromPeakImage plots the identified chromatographic peaks from one file into the plane spanned by the retention time and mz dimension (x-axis representing the retention time and y-axis mz). Each chromatographic peak is plotted as a rectangle representing its width in rt and mz dimension.

This plot is supposed to provide some initial overview of the chromatographic peak detection results.

plotChromPeakImage plots the number of detected peaks for each sample along the retention time axis as an *image* plot, i.e. with the number of peaks detected in each bin along the retention time represented with the color of the respective cell.

Usage

```
plotChromPeaks(x, file = 1, xlim = NULL, ylim = NULL, add = FALSE,
  border = "#00000060", col = NA, xlab = "retention time", ylab = "mz",
  main = NULL, ...)

plotChromPeakImage(x, binSize = 30, xlim = NULL, log = FALSE,
  xlab = "retention time", yaxt = par("yaxt"),
  main = "Chromatographic peak counts", ...)
```

Arguments

x	XCMSnExp object.
file	For plotChromPeaks: numeric(1) specifying the index of the file within x for which the plot should be created. Defaults to 1.
xlim	numeric(2) specifying the x-axis limits (retention time dimension). Defaults to NULL in which case the full retention time range of the file is used.
ylim	For plotChromPeaks: numeric(2) specifying the y-axis limits (mz dimension). Defaults to NULL in which case the full mz range of the file is used.
add	For plotChromPeaks: logical(1) whether the plot should be added or created as a new plot.
border	For plotChromPeaks: the color for the rectangles' border.
col	For plotChromPeaks: the color to be used to fill the rectangles.
xlab	character(1) defining the x-axis label.
ylab	For plotChromPeaks: character(1) defining the y-axis label.
main	character(1) defining the plot title. By default (i.e. main = NULL the name of the file will be used as title.

...	Additional arguments passed to the plot (for plotChromPeaks) and image (for plotChromPeakImage) functions. Ignored if add = TRUE.
binSize	For plotChromPeakImage: numeric(1) defining the size of the bins along the x-axis (retention time). Defaults to binSize = 30, peaks within each 30 seconds will thus counted and plotted.
log	For plotChromPeakImage: logical(1) whether the peak counts should be log2 transformed before plotting.
yaxt	For plotChromPeakImage: character(1) defining whether y-axis labels should be added. To disable the y-axis use yaxt = "n". For any other value of yaxt the axis will be drawn. See par help page for more details.

Details

The width and line type of the rectangles indicating the detected chromatographic peaks for the plotChromPeaks function can be specified using the par function, i.e. with par(lwd = 3) and par(lty = 2), respectively.

Author(s)

Johannes Rainer

See Also

highlightChromPeaks for the function to highlight detected chromatographic peaks in extracted ion chromatogram plots.

Examples

```
## Perform peak detection on two files from the faahKO package.
library(xcms)
library(faahKO)
faahko_file <- c(system.file('cdf/KO/ko16.CDF', package = "faahKO"),
                 system.file('cdf/KO/ko18.CDF', package = "faahKO"))

od <- readMSData(faahko_file, mode = "onDisk")

## Peak detection using the 'matchedFilter' method. Note that we are using a
## larger binSize to reduce the runtime of the example.
xod <- findChromPeaks(od, param = MatchedFilterParam(binSize = 0.3, snthresh = 20))

## plotChromPeakImage: plot an image for the identified peaks per file
plotChromPeakImage(xod)

## Show all detected chromatographic peaks from the first file
plotChromPeaks(xod)

## Plot all detected peaks from the second file and restrict the plot to a
## mz-rt slice
plotChromPeaks(xod, file = 2, xlim = c(3500, 3600), ylim = c(400, 600))
```

plotEIC-methods *Plot extracted ion chromatograms for specified m/z range*

Description

Plot extracted ion chromatogram for m/z values of interest. The raw data is used in contrast to `plotChrom` which uses data from the profile matrix.

Arguments

`object`	`xcmsRaw` object
`mzrange`	m/z range for EIC. Uses the full m/z range by default.
`rtrange`	retention time range for EIC. Uses the full retention time range by default.
`scanrange`	scan range for EIC
`mzdec`	Number of decimal places of title m/z values in the eic plot.
`type`	Speficies how the data should be plotted (by default as a line).
`add`	If the EIC should be added to an existing plot.
`...`	Additional parameters passed to the plotting function (e.g. `col` etc).

Value

A two-column matrix with the plotted points.

Methods

object = "xcmsRaw" `plotEIC(object, mzrange = numeric(), rtrange = numeric(), scanrange = nu`

Author(s)

Ralf Tautenhahn

See Also

`rawEIC`, `xcmsRaw-class`

plotMsData *Create a plot that combines a XIC and a mz/rt 2D plot for one sample*

Description

The `plotMsData` creates a plot that combines an (base peak) extracted ion chromatogram on top (rt against intensity) and a plot of rt against m/z values at the bottom.

Usage

```
plotMsData(x, main = "", cex = 1, mfrow = c(2, 1),
  grid.color = "lightgrey", colramp = colorRampPalette(rev(brewer.pal(9,
  "YlGnBu"))))
```

Arguments

x	data.frame such as returned by the extractMsData() function. Only a single data.frame is supported.
main	character(1) specifying the title.
cex	numeric(1) defining the size of points. Passed directly to the plot function.
mfrow	numeric(2) defining the plot layout. This will be passed directly to par(mfrow = mfrow). See par for more information. Setting mfrow = NULL avoids calling par(mfrow = mfrow) hence allowing to pre-define the plot layout.
grid.color	a color definition for the grid line (or NA to skip creating them).
colramp	a *color ramp palette* to be used to color the data points based on their intensity. See argument col.regions in lattice::level.colors documentation.

Author(s)

Johannes Rainer

See Also

extractMsData() for the method to extract the data to plot.

Examples

```
## Read two files from the faahKO package
library(faahKO)
cdfs <- dir(system.file("cdf", package = "faahKO"), full.names = TRUE,
    recursive = TRUE)[1:2]
raw_data <- readMSData(cdfs, mode = "onDisk")
## Extract the MS data from a slice of data
msd <- extractMsData(raw_data, mz = c(334.9, 335.1), rt = c(2700, 2900))

## Plot the data for the first file
plotMsData(msd[[1]])

## To plot the data for both files:
layout(mat = matrix(1:4, ncol = 2))
plotMsData(msd[[1]], mfrow = NULL)
plotMsData(msd[[2]], mfrow = NULL)
```

---

plotPeaks-methods *Plot a grid of a large number of peaks*

Description

Plot extracted ion chromatograms for many peaks simultaneously, indicating peak integration start and end points with vertical grey lines.

Arguments

object	the xcmsRaw object
peaks	matrix with peak information as produced by findPeaks
figs	two-element vector describing the number of rows and the number of columns of peaks to plot, if missing then an approximately square grid that will fit the number of peaks supplied
width	width of chromatogram retention time to plot for each peak

Details

This function is intended to help graphically analyze the results of peak picking. It can help estimate the number of false positives and improper integration start and end points. Its output is very compact and tries to waste as little space as possible. Each plot is labeled with rounded m/z and retention time separated by a space.

Methods

object = "xcmsRaw" `plotPeaks(object, peaks, figs, width = 200)`

See Also

xcmsRaw-class, findPeaks, split.screen

---

plotQC — *Plot m/z and RT deviations for QC purposes without external reference data*

Description

Use "democracy" to determine the average m/z and RT deviations for a grouped xcmsSet, and dependency on sample or absolute m/z

Usage

```
plotQC(object, sampNames, sampColors, sampOrder, what)
```

Arguments

object	A grouped xcmsSet
sampNames	Override sample names (e.g. with simplified names)
sampColors	Provide a set of colors (default: monochrome ?)
sampOrder	Override the order of samples, e.g. to bring them in order of measurement to detect time drift
what	A vector of which QC plots to generate. "mzdevhist": histogram of mz deviations. Should be gaussian shaped. If it is multimodal, then some peaks seem to have a systematically higher m/z deviation "rtdevhist": histogram of RT deviations. Should be gaussian shaped. If it is multimodal, then some peaks seem to have a systematically higher RT deviation "mzdevmass": Shows whether m/z deviations are absolute m/z dependent, could indicate miscalibration "mzdevtime": Shows whether m/z deviations are RT dependent, could indicate instrument drift "mzdevsample": median mz deviation for each sample, indicates outliers "rtdevsample": median RT deviation for each sample, indicates outliers

Details

plotQC() is a warpper to create a set of diagnostic plots. For the m/z deviations, the median of all m/z withon one group are assumed.

Value

List with four matrices, each of dimension features * samples: "mz": median mz deviation for each sample "mzdev": median mz deviation for each sample "rt": median RT deviation for each sample "rtdev": median RT deviation for each sample

Author(s)

Michael Wenk, Michael Wenk <michael.wenk@student.uni-halle.de>

Examples

```
library(faahKO)
xsg <- group(faahko)

plotQC(xsg, what="mzdevhist")
plotQC(xsg, what="rtdevhist")
plotQC(xsg, what="mzdevmass")
plotQC(xsg, what="mzdevtime")
plotQC(xsg, what="mzdevsample")
plotQC(xsg, what="rtdevsample")
```

---

plotRaw-methods *Scatterplot of raw data points*

Description

Produce a scatterplot showing raw data point location in retention time and m/z. This plot is more useful for centroided data than continuum data.

Arguments

object	the xcmsRaw object
mzrange	numeric vector of length >= 2 whose range will be used to select the masses to plot
rtrange	numeric vector of length >= 2 whose range will be used to select the retention times to plot
scanrange	numeric vector of length >= 2 whose range will be used to select scans to plot
log	logical, log transform intensity
title	main title of the plot

Value

A matrix with the points plotted.

Methods

object = "xcmsRaw" `plotRaw(object, mzrange = numeric(), rtrange = numeric(), scanrange`

See Also

xcmsRaw-class

---

plotrt-methods *Plot retention time deviation profiles*

Description

Use corrected retention times for each sample to calculate retention time deviation profiles and plot each on the same graph.

Arguments

object	the xcmsSet object
col	vector of colors for plotting each sample
ty	vector of line and point types for plotting each sample
leg	logical plot legend with sample labels
densplit	logical, also plot peak overall peak density

Methods

object = "xcmsSet" `plotrt(object, col = NULL, ty = NULL, leg = TRUE, densplit = FALSE)`

See Also

xcmsSet-class, retcor

---

plotScan-methods *Plot a single mass scan*

Description

Plot a single mass scan using the impulse representation. Most useful for centroided data.

Arguments

object	the xcmsRaw object
scan	integer with number of scan to plot
mzrange	numeric vector of length >= 2 whose range will be used to select masses to plot
ident	logical, use mouse to interactively identify and label individual masses

Methods

object = "xcmsRaw" `plotScan(object, scan, mzrange = numeric(), ident = FALSE)`

See Also

xcmsRaw-class

---

plotSpec-methods *Plot mass spectra from the profile matrix*

Description

Uses the pre-generated profile mode matrix to plot mass spectra over a specified retention time range.

Arguments

object	the xcmsRaw object
ident	logical, use mouse to identify and label peaks
vline	numeric vector with locations of vertical lines
...	arguments passed to profRange

Value

If ident == TRUE, an integer vector with the indecies of the points that were identified. Otherwise a two-column matrix with the plotted points.

Methods

object = "xcmsRaw" plotSpec(object, ident = FALSE, vline = numeric(0), ...)

See Also

xcmsRaw-class

---

plotSurf-methods *Plot profile matrix 3D surface using OpenGL*

Description

This method uses the rgl package to create interactive three dimensonal representations of the profile matrix. It uses the terrain color scheme.

Arguments

object	the xcmsRaw object
log	logical, log transform intensity
aspect	numeric vector with aspect ratio of the m/z, retention time and intensity components of the plot
...	arguments passed to profRange

Details

The rgl package is still in development and imposes some limitations on the output format. A bug in the axis label code means that the axis labels only go from 0 to the aspect ratio constant of that axis. Additionally the axes are not labeled with what they are.

It is important to only plot a small portion of the profile matrix. Large portions can quickly overwhelm your CPU and memory.

Methods

object = "xcmsRaw" `plotSurf(object, log = FALSE, aspect = c(1, 1, .5), ...)`

See Also

xcmsRaw-class

`plotTIC-methods` *Plot total ion count*

Description

Plot chromatogram of total ion count. Optionally allow identification of target peaks and viewing/identification of individual spectra.

Arguments

`object`	the `xcmsRaw` object
`ident`	logical, use mouse to identify and label chromatographic peaks
`msident`	logical, use mouse to identify and label spectral peaks

Value

If `ident == TRUE`, an integer vector with the indecies of the points that were identified. Otherwise a two-column matrix with the plotted points.

Methods

object = "xcmsRaw" `plotTIC(object, ident = FALSE, msident = FALSE)`

See Also

xcmsRaw-class

`ProcessHistory-class` *Tracking data processing*

Description

Objects of the type `ProcessHistory` allow to keep track of any data processing step in an metabolomics experiment. They are created by the data processing methods, such as `findChromPeaks` and added to the corresponding results objects. Thus, usually, users don't need to create them.

The `XProcessHistory` extends the `ProcessHistory` by adding a slot `param` that allows to store the actual parameter class of the processing step.

`processParam`, `processParam<-`: get or set the parameter class from an `XProcessHistory` object.

`msLevel`: returns the MS level on which a certain analysis has been performed, or `NA` if not defined.

The `processType` method returns a character specifying the processing step *type*.

The `processDate` extracts the start date of the processing step.

The `processInfo` extracts optional additional information on the processing step.

The `fileIndex` extracts the indices of the files on which the processing step was applied.

Usage

```
## S4 method for signature 'ProcessHistory'
show(object)

## S4 method for signature 'XProcessHistory'
show(object)

## S4 method for signature 'XProcessHistory'
processParam(object)

## S4 method for signature 'XProcessHistory'
msLevel(object)

## S4 method for signature 'ProcessHistory'
processType(object)

## S4 method for signature 'ProcessHistory'
processDate(object)

## S4 method for signature 'ProcessHistory'
processInfo(object)

## S4 method for signature 'ProcessHistory'
fileIndex(object)
```

Arguments

`object`	A `ProcessHistory` or `XProcessHistory` object.

Value

For `processParam`: a parameter object extending the `Param` class.

The `processType` method returns a character string with the processing step type.

The `processDate` method returns a character string with the time stamp of the processing step start.

The `processInfo` method returns a character string with optional additional informations.

The `fileIndex` method returns a integer vector with the index of the files/samples on which the processing step was applied.

Slots

`type` character(1): string defining the type of the processing step. This string has to match predefined values. Use `processHistoryTypes` to list them.

`date` character(1): date time stamp when the processing step was started.

`info` character(1): optional additional information.

`fileIndex` integer of length 1 or > 1 to specify on which samples of the object the processing was performed.

`error` (ANY): used to store eventual calculation errors.

`param` (Param): an object of type `Param` (e.g. `CentWaveParam`) specifying the settings of the processing step.

`msLevel:` `integer` defininining the MS level(s) on which the analysis was performed.

Author(s)

Johannes Rainer

`profMat-xcmsSet` *The profile matrix*

Description

The *profile* matrix is an n x m matrix, n (rows) representing equally spaced m/z values (bins) and m (columns) the retention time of the corresponding scans. Each cell contains the maximum intensity measured for the specific scan and m/z values falling within the m/z bin.

The `profMat` method creates a new profile matrix or returns the profile matrix within the object's `@env` slot, if available. Settings for the profile matrix generation, such as `step` (the bin size), `method` or additional settings are extracted from the respective slots of the `xcmsRaw` object. Alternatively it is possible to specify all of the settings as additional parameters.

Usage

```
## S4 method for signature 'xcmsRaw'
profMat(object, method, step, baselevel, basespace,
  mzrange.)
```

Arguments

object	The xcmsRaw object.
method	The profile matrix generation method. Allowed are "bin", "binlin", "binlinbase" and "intlin". See details section for more information.
step	numeric(1) representing the m/z bin size.
baselevel	numeric(1) representing the base value to which empty elements (i.e. m/z bins without a measured intensity) should be set. Only considered if method = "binlinbase". See baseValue parameter of imputeLinInterpol for more details.
basespace	numeric(1) representing the m/z length after which the signal will drop to the base level. Linear interpolation will be used between consecutive data points falling within 2 * basespace to each other. Only considered if method = "binlinbase". If not specified, it defaults to 0.075. Internally this parameter is translated into the distance parameter of the imputeLinInterpol function by distance = floor(basespace / s See distance parameter of imputeLinInterpol for more details.
mzrange.	Optional numeric(2) manually specifying the mz value range to be used for binnind. If not provided, the whole mz value range is used.

Details

Profile matrix generation methods:

bin The default profile matrix generation method that does a simple binning, i.e. aggregating of intensity values falling within an m/z bin.

binlin Binning followed by linear interpolation to impute missing values. The value for m/z bins without a measured intensity are inferred by a linear interpolation between neighboring bins with a measured intensity.

binlinbase Binning followed by a linear interpolation to impute values for empty elements (m/z bins) within a user-definable proximity to non-empty elements while stetting the element's value to the baselevel otherwise. See impute = "linbase" parameter of imputeLinInterpol for more details.

intlin Set the elements' values to the integral of the linearly interpolated data from plus to minus half the step size.

Value

profMat returns the profile matrix (rows representing scans, columns equally spaced m/z values).

Note

From xcms version 1.51.1 on only the profMat method should be used to extract the profile matrix instead of the previously default way to access it directly *via* object@env$profile.

Author(s)

Johannes Rainer

See Also

xcmsRaw, binYonX and imputeLinInterpol for the employed binning and missing value imputation methods, respectively. profMat,XCMSnExp-method for the method on XCMSnExp objects.

Examples

```
file <- system.file('cdf/KO/ko15.CDF', package = "faahKO")
## Load the data without generating the profile matrix (profstep = 0)
xraw <- xcmsRaw(file, profstep = 0)
## Extract the profile matrix
profmat <- profMat(xraw, step = 0.3)
dim(profmat)
## If not otherwise specified, the settings from the xraw object are used:
profinfo(xraw)
## To extract a profile matrix with linear interpolation use
profmat <- profMat(xraw, step = 0.3, method = "binlin")
## Alternatively, the profMethod of the xraw objects could be changed
profMethod(xraw) <- "binlin"
profmat_2 <- profMat(xraw, step = 0.3)
all.equal(profmat, profmat_2)
```

---

profMedFilt-methods *Median filtering of the profile matrix*

Description

Apply a median filter of given size to a profile matrix.

Arguments

object	the xcmsRaw object
massrad	number of m/z grid points on either side to use for median calculation
scanrad	number of scan grid points on either side to use for median calculation

Methods

object = "xcmsRaw" `profMedFilt(object, massrad = 0, scanrad = 0)`

See Also

xcmsRaw-class, medianFilter

---

profMethod-methods *Get and set method for generating profile data*

Description

These methods get and set the method for generating profile (matrix) data from raw mass spectral data. It can currently be bin, binlin, binlinbase, or intlin.

Methods

object = "xcmsRaw" `profMethod(object)`

See Also

xcmsRaw-class, profMethod, profBin, plotSpec, plotChrom, findPeaks

profRange-methods *Specify a subset of profile mode data*

Description

Specify a subset of the profile mode matrix given a mass, time, or scan range. Allow flexible user entry for other functions.

Arguments

object	the xcmsRaw object
mzrange	single numeric mass or vector of masses
rtrange	single numeric time (in seconds) or vector of times
scanrange	single integer scan index or vector of indecies
...	arguments to other functions

Details

This function handles selection of mass/time subsets of the profile matrix for other functions. It allows the user to specify such subsets in a variety of flexible ways with minimal typing.

Because R does partial argument matching, mzrange, scanrange, and rtrange can be specified in short form using m=, s=, and t=, respectively. If both a scanrange and rtrange are specified, then the rtrange specification takes precedence.

When specifying ranges, you may either enter a single number or a numeric vector. If a single number is entered, then the closest single scan or mass value is selected. If a vector is entered, then the range is set to the range() of the values entered. That allows specification of ranges using shortened, slightly non-standard syntax. For example, one could specify 400 to 500 seconds using any of the following: t=c(400,500), t=c(500,400), or t=400:500. Use of the sequence operator (:) can save several keystrokes when specifying ranges. However, while the sequence operator works well for specifying integer ranges, fractional ranges do not always work as well.

Value

A list with the folloing items:

mzrange	numeric vector with start and end mass
masslab	textual label of mass range
massidx	integer vector of mass indecies
scanrange	integer vector with stat ane end scans
scanlab	textual label of scan range
scanidx	integer vector of scan range
rtrange	numeric vector of start and end times
timelab	textual label of time range

Methods

object = "xcmsRaw" profRange(object, mzrange = numeric(), rtrange = numeric(), scanr

See Also

xcmsRaw-class

---

profStep-methods *Get and set m/z step for generating profile data*

Description

These methods get and set the m/z step for generating profile (matrix) data from raw mass spectral data. Smaller steps yield more precision at the cost of greater memory usage.

Methods

object = "xcmsRaw" profStep(object)

See Also

xcmsRaw-class, profMethod

Examples

```
## Not run:
library(faahKO)
cdfpath <- system.file("cdf", package = "faahKO")
cdffiles <- list.files(cdfpath, recursive = TRUE, full.names = TRUE)
xset <- xcmsRaw(cdffiles[1])

xset
plotSurf(xset, mass=c(200,500))

profStep(xset)<-0.1 ## decrease the bin size to get better resolution
plotSurf(xset, mass=c(200, 500))
##works nicer on high resolution data.

## End(Not run)
```

---

rawEIC-methods *Get extracted ion chromatograms for specified m/z range*

Description

Generate extracted ion chromatogram for m/z values of interest. The raw data is used in contrast to getEIC which uses data from the profile matrix (i.e. values binned along the M/Z dimension).

Arguments

object	xcmsRaw object
mzrange	m/z range for EIC
rtrange	retention time range for EIC
scanrange	scan range for EIC

Value

A list of :

scan	scan number
intensity	added intensity values

Methods

object = "xcmsRaw" `rawEIC(object, mzrange = numeric(), rtrange = numeric(), scanrange = numeri`

Author(s)

Ralf Tautenhahn

See Also

xcmsRaw-class

---

rawMat-methods *Get a raw data matrix*

Description

Returns a matrix with columns for time, m/z, and intensity that represents the raw data from a chromatography mass spectrometry experiment.

Arguments

object	The container of the raw data
mzrange	Subset by m/z range
rtrange	Subset by retention time range
scanrange	Subset by scan index range
log	Whether to log transform the intensities

Value

A numeric matrix with three columns: time, mz and intensity.

Methods

object = "xcmsRaw" `rawMat(object, mzrange = numeric(), rtrange = numeric(), scanrange = numeri`

Author(s)

Michael Lawrence

See Also

plotRaw for plotting the raw intensities

retcor-methods *Correct retention time from different samples*

Description

To correct differences between retention times between different samples, a number of of methods exist in XCMS. `retcor` is the generic method.

Arguments

`object`	`xcmsSet-class` object
`method`	Method to use for retention time correction. See details.
`...`	Optional arguments to be passed along

Details

Different algorithms can be used by specifying them with the `method` argument. For example to use the approach described by Smith et al (2006) one would use: `retcor(object, method="loess")`. This is also the default.

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

A character vector of *nicknames* for the algorithms available is returned by `getOption("BioC")$xcms$retcor.methods` If the nickname of a method is called "loess", the help page for that specific method can be accessed with `?retcor.loess`.

Value

An `xcmsSet` object with corrected retntion times.

Methods

object = "xcmsSet" `retcor(object, ...)`

See Also

`retcor.loess` `retcor.obiwarp` `xcmsSet-class`,

retcor.obiwarp *Align retention times across samples with Obiwarp*

Description

Calculate retention time deviations for each sample. It is based on the code at `http://obi-warp.sourceforge.net/`. However, this function is able to align multiple samples, by a center-star strategy.

For the original publication see

Chromatographic Alignment of ESI-LC-MS Proteomics Data Sets by Ordered Bijective Interpolated Warping John T. Prince and, Edward M. Marcotte Analytical Chemistry 2006 78 (17), 6140-6152

Arguments

object	the xcmsSet object
plottype	if deviation plot retention time deviation
profStep	step size (in m/z) to use for profile generation from the raw data files
center	the index of the sample all others will be aligned to. If center==NULL, the sample with the most peaks is chosen as default.
col	vector of colors for plotting each sample
ty	vector of line and point types for plotting each sample
response	Responsiveness of warping. 0 will give a linear warp based on start and end points. 100 will use all bijective anchors
distFunc	DistFunc function: cor (Pearson's R) or cor_opt (default, calculate only 10% diagonal band of distance matrix, better runtime), cov (covariance), prd (product), euc (Euclidean distance)
gapInit	Penalty for Gap opening, see below
gapExtend	Penalty for Gap enlargement, see below
factorDiag	Local weighting applied to diagonal moves in alignment.
factorGap	Local weighting applied to gap moves in alignment.
localAlignment	Local rather than global alignment
initPenalty	Penalty for initiating alignment (for local alignment only) Default: 0 Default gap penalties: (gapInit, gapExtend) [by distFunc type]: 'cor' = '0.3,2.4' 'cov' = '0,11.7' 'prd' = '0,7.8' 'euc' = '0.9,1.8'

Value

An xcmsSet object

Methods

object = "xcmsSet" retcor(object, method="obiwarp", plottype = c("none", "deviation"), profStep=1, center=NULL, col = NULL, ty = NULL, response=1, distFunc="cor_opt", gapInit=NULL, gapExtend=NULL, factorDiag=2, factorGap=1, localAlignment=0, initPenalty=0)

See Also

xcmsSet-class,

---

retcor.peakgroups-methods

Align retention times across samples

Description

These two methods use "well behaved" peak groups to calculate retention time deviations for every time point of each sample. Use smoothed deviations to align retention times.

Arguments

object	the xcmsSet object
missing	number of missing samples to allow in retention time correction groups
extra	number of extra peaks to allow in retention time correction correction groups
smooth	either "loess" for non-linear alignment or "linear" for linear alignment
span	degree of smoothing for local polynomial regression fitting
family	if gaussian fitting is by least-squares with no outlier removal, and if symmetric a re-descending M estimator is used with Tukey's biweight function, allowing outlier removal
plottype	if deviation plot retention time deviation points and regression fit, and if mdevden also plot peak overall peak density and retention time correction peak density
col	vector of colors for plotting each sample
ty	vector of line and point types for plotting each sample

Value

An xcmsSet object

Methods

object = "xcmsSet" `retcor(object, missing = 1, extra = 1, smooth = c("loess", "linear"),`

See Also

xcmsSet-class, loess retcor.obiwarp

---

retexp *Set retention time window to a specified width*

Description

Expands (or contracts) the retention time window in each row of a matrix as defined by the retmin and retmax columns.

Usage

```
retexp(peakrange, width = 200)
```

Arguments

peakrange	maxtrix with columns retmin and retmax
width	new width for the window

Value

The altered matrix.

Author(s)

Colin A. Smith, <csmith@scripps.edu>

See Also

getEIC

---

sampnames-methods *Get sample names*

Description

Return sample names for an object

Value

A character vector with sample names.

Methods

object = "xcmsEIC" sampnames(object)
object = "xcmsSet" sampnames(object)

See Also

xcmsSet-class, xcmsEIC-class

---

showError,xcmsSet-method
Extract processing errors

Description

If peak detection is performed with findPeaks setting argument stopOnError = FALSE eventual errors during the process do not cause to stop the processing but are recorded inside of the resulting xcmsSet object. These errors can be accessed with the showError method.

Usage

```
## S4 method for signature 'xcmsSet'
showError(object, message. = TRUE, ...)
```

Arguments

object	An xcmsSet object.
message.	Logical indicating whether only the error message, or the error itself should be returned.
...	Additional arguments.

Value

A list of error messages (if message. = TRUE) or errors or an empty list if no errors are present.

Author(s)

Johannes Rainer

specDist-methods *Distance methods for xcmsSet, xcmsRaw and xsAnnotate*

Description

There are several methods for calculating a distance between two sets of peaks in xcms. specDist is the generic method.

Arguments

object	a xcmsSet or xcmsRaw.
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 with xcmsSet one would use: specDist(object, peakIDs1, peakIDs2, method="mea This is also the default.

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

A character vector of *nicknames* for the algorithms available is returned by getOption("BioC")$xcms$specDist.metho 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

object = "xcmsSet" specDist(object, peakIDs1, peakIDs2,...)

object = "xsAnnotate" specDist(object, PSpec1, PSpec2,...)

Author(s)

Joachim Kutzera, <jkutzer@ipb-halle.de>

specDist.cosine *a Distance function based on matching peaks*

Description

This method calculates the distance of two sets of peaks using the cosine-distance.

Usage

```
specDist.cosine(peakTable1, peakTable2, mzabs=0.001, mzppm=10, mzExp=0.6, intExp=3, nPdiff=2, nPm
```

Arguments

peakTable1	a Matrix containing at least m/z-values, row must be called "mz"
peakTable2	the matrix for the other mz-values
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
mzExp	the exponent used for mz
intExp	the exponent used for intensity
nPdiff	the maximum nrow-difference of the two peaktables
nPmin	the minimum absolute sum of peaks from both praktables

Details

The result is the cosine-distance of the product from weighted factors of mz and intensity from matching peaks in the two peaktables. The factors are calculated as wFact = mz^mzExp * int^intExp. if no distance is calculated (for example because no matching peaks were found) the return-value is NA.

Methods

peakTable1 = "matrix", peakTable2 = "matrix" `specDist.cosine(peakTable1, peakTable2, mzabs = 0.0`

Author(s)

Joachim Kutzera, <jkutzer@ipb-halle.de>

specDist.meanMZmatch *a Distance function based on matching peaks*

Description

This method calculates the distance of two sets of peaks.

Usage

```
specDist.meanMZmatch(peakTable1, peakTable2, matchdist=1, matchrate=1, mzabs=0.001, mzppm=10, sym
```

Arguments

peakTable1	a Matrix containing at least m/z-values, row must be called "mz"
peakTable2	the matrix for the other mz-values
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
matchdist	the weight for value one (see details)
matchrate	the weight for value two

Details

The result of the calculation is a weighted sum of two values. Value one is the mean absolute difference of the matching peaks, value two is the relation of matching peaks and non matching peaks. if no distance is calculated (for example because no matching peaks were found) the return-value is NA.

Methods

peakTable1 = "matrix", peakTable2 = "matrix" `specDist.meanMZmatch(peakTable1, peakTable2, mat`

Author(s)

Joachim Kutzera, <jkutzer@ipb-halle.de>

specDist.peakCount-methods
a Distance function based on matching peaks

Description

This method calculates the distance of two sets of peaks by just returning the number of matching peaks (m/z-values).

Usage

```
specDist.peakCount(peakTable1, peakTable2, mzabs=0.001, mzppm=10, symmetric=FALSE)
```

Arguments

peakTable1	a Matrix containing at least m/z-values, row must be called "mz"
peakTable2	the matrix for the other mz-values
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

peakTable1 = "matrix", peakTable2 = "matrix" `specDist.peakCount(peakTable1, peakTable2, mzppm=1`

Author(s)

Joachim Kutzera, <jkutzer@ipb-halle.de>

---

specNoise *Calculate noise for a sparse continuum mass spectrum*

Description

Given a sparse continuum mass spectrum, determine regions where no signal is present, substituting half of the minimum intensity for those regions. Calculate the noise level as the weighted mean of the regions with signal and the regions without signal. If there is only one raw peak, return zero.

Usage

```
specNoise(spec, gap = quantile(diff(spec[, "mz"]), 0.9))
```

Arguments

spec	matrix with named columns mz and intensity
gap	threshold above which to data points are considerd to be separated by a blank region and not bridged by an interpolating line

Details

The default gap value is determined from the 90th percentile of the pair-wise differences between adjacent mass values.

Value

A numeric noise level

Author(s)

Colin A. Smith, <csmith@scripps.edu>

See Also

getSpec, specPeaks

specPeaks *Identify peaks in a sparse continuum mode spectrum*

Description

Given a spectrum, identify and list significant peaks as determined by several criteria.

Usage

```
specPeaks(spec, sn = 20, mzgap = 0.2)
```

Arguments

spec	matrix with named columns mz and intensity
sn	minimum signal to noise ratio
mzgap	minimal distance between adjacent peaks, with smaller peaks being excluded

Details

Peaks must meet two criteria to be considered peaks: 1) Their s/n ratio must exceed a certain threshold. 2) They must not be within a given distance of any greater intensity peaks.

Value

A matrix with columns:

mz	m/z at maximum peak intensity
intensity	maximum intensity of the peak
fwhm	full width at half max of the peak

Author(s)

Colin A. Smith, <csmith@scripps.edu>

See Also

getSpec, specNoise

split.xcmsRaw *Divide an xcmsRaw object*

Description

Divides the scans from a xcmsRaw object into a list of multiple objects. MS^n data is discarded.

Arguments

x	xcmsRaw object
f	factor such that factor(f) defines the scans which go into the new xcmsRaw objects
drop	logical indicating if levels that do not occur should be dropped (if 'f' is a 'factor' or a list).
...	further potential arguments passed to methods.

Value

A list of xcmsRaw objects.

Methods

xr = "xcmsRaw" `split(x, f, drop = TRUE, ...)`

Author(s)

Steffen Neumann, <sneumann(at)ipb-halle.de>

See Also

xcmsRaw-class

split.xcmsSet *Divide an xcmsSet object*

Description

Divides the samples and peaks from a xcmsSet object into a list of multiple objects. Group data is discarded.

Arguments

xs	xcmsSet object
f	factor such that factor(f) defines the grouping
drop	logical indicating if levels that do not occur should be dropped (if 'f' is a 'factor' or a list).
...	further potential arguments passed to methods.

Value

A list of xcmsSet objects.

Methods

xs = "xcmsSet" split(x, f, drop = TRUE, ...)

Author(s)

Colin A. Smith, <csmith@scripps.edu>

See Also

xcmsSet-class

SSgauss *Gaussian Model*

Description

This selfStart model evalueates the Gaussian model and its gradient. It has an initial attribute that will evalueate the inital estimates of the parameters mu, sigma, and h.

Usage

```
SSgauss(x, mu, sigma, h)
```

Arguments

x	a numeric vector of values at which to evaluate the model
mu	mean of the distribution function
sigma	standard deviation of the distribution fuction
h	height of the distribution function

Details

Initial values for mu and h are chosen from the maximal value of x. The initial value for sigma is determined from the area under x divided by h*sqrt(2*pi).

Value

A numeric vector of the same length as x. It is the value of the expression h*exp(-(x-mu)^2/(2*sigma^2), which is a modified gaussian function where the maximum height is treated as a separate parameter not dependent on sigma. If arguments mu, sigma, and h are names of objects, the gradient matrix with respect to these names is attached as an attribute named gradient.

Author(s)

Colin A. Smith, <csmith@scripps.edu>

See Also

nls, selfStart

stitch-methods *Correct gaps in data*

Description

Fixes gaps in data due to calibration scans or lock mass. Automatically detects file type and calls the relevant method. The mzXML file keeps the data the same length in time but overwrites the lock mass scans. The netCDF version adds the scans back into the data thereby increasing the length of the data and correcting for the unseen gap.

Arguments

object	An xcmsRaw-class object
lockMass	A dataframe of locations of the gaps
freq	The intervals of the lock mass scans
start	The starting lock mass scan location, default is 1

Details

makeacqNum takes locates the gap using the starting lock mass scan and it's intervals. This data frame is then used in stitch to correct for the gap caused by the lock mass. Correction works by using scans from either side of the gap to fill it in.

Value

stitch A corrected xcmsRaw-class object makeacqNum A numeric vector of scan locations corresponding to lock Mass scans

Methods

object = "xcmsRaw" `stitch(object, lockMass=numeric())`

object = "xcmsRaw" `makeacqNum(object, freq=numeric(), start=1)`

Author(s)

Paul Benton, <hpaul.benton08@imperial.ac.uk>

Examples

```
## Not run: library(xcms)
library(faahKO) ## These files do not have this problem to correct for but just for an example
cdfpath <- system.file("cdf", package = "faahKO")
cdffiles <- list.files(cdfpath, recursive = TRUE, full.names = TRUE)
xr<-xcmsRaw(cdffiles[1])
xr
##Lets assume that the lockmass starts at 1 and is every 100 scans
lockMass<-xcms:::makeacqNum(xr, freq=100, start=1)
## these are equcal
lockmass<-AutoLockMass(xr)
ob<-stitch(xr, lockMass)
ob
```

```
#plot the old data before correction
foo<-rawEIC(xr, m=c(200,210), scan=c(80,140))
plot(foo$scan, foo$intensity, type="h")

#plot the new corrected data to see what changed
foo<-rawEIC(ob, m=c(200,210), scan=c(80,140))
plot(foo$scan, foo$intensity, type="h")

## End(Not run)
```

---

updateObject,xcmsSet-method *Update an* xcmsSet *object*

Description

This method updates an *old* xcmsSet object to the latest definition.

Usage

```
## S4 method for signature 'xcmsSet'
updateObject(object, ..., verbose = FALSE)
```

Arguments

object	The xcmsSet object to update.
...	Optional additional arguments. Currently ignored.
verbose	Currently ignored.

Value

An updated xcmsSet containing all data from the input object.

Author(s)

Johannes Rainer

---

useOriginalCode *Enable usage of old xcms code*

Description

This function allows to enable the usage of old, partially deprecated code from xcms by setting a corresponding global option. See details for functions affected.

Usage

```
useOriginalCode(x)
```

Arguments

x	logical(1) to specify whether or not original old code should be used in corresponding functions. If not provided the function simply returns the value of the global option.

Details

The functions/methods that will be affected by this are:

- do_findChromPeaks_matchedFilter

Value

logical(1) indicating whether old code is being used.

Note

Usage of old code is strongly dicouraged. This function is thought to be used mainly in the transition phase from xcms to xcms version 3.

Author(s)

Johannes Rainer

---

verify.mzQuantM *Verify an mzQuantML file*

Description

Export in XML data formats: verify the written data

Usage

```
verify.mzQuantML(filename, xsdfilename)
```

Arguments

filename	filename (may include full path) for the output file. Pipes or URLs are not allowed.
xsdfilename	Filename of the XSD to verify against (may include full path)

Details

The verify.mzQuantML() function will verify an PSI standard format mzQuantML document against the XSD schemda, see http://www.psidev.info/mzquantml

Value

None.

See Also

write.mzQuantML

write.cdf-methods *Save an xcmsRaw object to file*

Description

Write the raw data to a (simple) CDF file.

Arguments

object	the xcmsRaw object
filename	filename (may include full path) for the CDF file. Pipes or URLs are not allowed.

Details

Currently the only application known to read the resulting file is XCMS. Others, especially those which build on the AndiMS library, will refuse to load the output.

Value

None.

Methods

object = "xcmsRaw" `write.cdf(object, filename)`

See Also

xcmsRaw-class, xcmsRaw,

write.mzdata-methods *Save an xcmsRaw object to a file*

Description

Write the raw data to a (simple) mzData file.

Arguments

object	the xcmsRaw object
filename	filename (may include full path) for the mzData file. Pipes or URLs are not allowed.

Details

This function will export a given xcmsRaw object to an mzData file. The mzData file will contain a <spectrumList> containing the <spectrum> with mass and intensity values in 32 bit precision. Other formats are currently not supported. Any header information (e.g. additional <software> information or <cvParams>) will be lost. Currently, also any MSn information will not be stored.

Value

None.

Methods

object = "xcmsRaw" `write.mzdata(object, filename)`

See Also

xcmsRaw-class, xcmsRaw,

`write.mzQuantML-methods`

Save an xcmsSet object to an PSI mzQuantML file

Description

Export in XML data formats: Write the processed data in an xcmsSet to mzQuantML.

Arguments

`object`	the `xcmsRaw` or `xcmsSet` object
`filename`	filename (may include full path) for the output file. Pipes or URLs are not allowed.

Details

The write.mzQuantML() function will write a (grouped) xcmsSet into the PSI standard format mzQuantML, see http://www.psidev.info/mzquantml

Value

None.

Methods

object = "xcmsSet" `write.mzQuantML(object, filename)`

See Also

xcmsSet-class, xcmsSet, verify.mzQuantML,

writeMzTab *Save a grouped xcmsSet object in mzTab-1.1 format file*

Description

Write the grouped xcmsSet to an mzTab file.

Arguments

object	the xcmsSet object
filename	filename (may include full path) for the mzTab file. Pipes or URLs are not allowed.

Details

The mzTab file format for MS-based metabolomics (and proteomics) is a lightweight supplement to the existing standard XML-based file formats (mzML, mzIdentML, mzQuantML), providing a comprehensive summary, similar in concept to the supplemental material of a scientific publication. mzTab files from xcms contain small molecule sections together with experimental metadata and basic quantitative information. The format is intended to store a simple summary of the final results.

Value

None.

Usage

object = "xcmsSet" `writeMzTab(object, filename)`

See Also

xcmsSet-class, xcmsSet,

Examples

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

mzt <- data.frame(character(0))
mzt <- xcms:::mzTabHeader(mzt,
                  version="1.1.0", mode="Complete", type="Quantification",
                  description="faahKO",
                  xset=xs)
mzt <- xcms:::mzTabAddSME(mzt, xs)

xcms:::writeMzTab(mzt, "faahKO.mzTab")
```

xcms-deprecated *Deprecated functions in package 'xcms'*

Description

These functions are provided for compatibility with older versions of 'xcms' only, and will be defunct at the next release.

Details

The following functions/methods are deprecated.

- xcmsPapply: this function is no longer available and the use of bplapply is suggested.
- profBin, profBinM, profBinLin, profBinLinM, profBinLinBase, profBinLinBaseM have been deprecated and binYonX in combination with imputeLinInterpol should be used instead.
- extractChromatograms: replaced by chromatogram.
- plotChromatogram: replaced by plot method for Chromatogram or Chromatograms objects.

xcmsEIC-class *Class xcmsEIC, a class for multi-sample extracted ion chromatograms*

Description

This class is used to store and plot parallel extracted ion chromatograms from multiple sample files. It integrates with the xcmsSet class to display peak area integrated during peak identification or fill-in.

Objects from the Class

Objects can be created with the getEIC method of the xcmsSet class. Objects can also be created by calls of the form new("xcmsEIC", ...).

Slots

eic: list containing named entries for every sample. for each entry, a list of two column EIC matricies with retention time and intensity

mzrange: two column matrix containing starting and ending m/z for each EIC

rtrange: two column matrix containing starting and ending time for each EIC

rt: either "raw" or "corrected" to specify retention times contained in the object

groupnames: group names from xcmsSet object used to generate EICs

Methods

groupnames signature(object = "xcmsEIC"): get groupnames slot

mzrange signature(object = "xcmsEIC"): get mzrange slot

plot signature(x = "xcmsEIC"): plot the extracted ion chromatograms

rtrange signature(object = "xcmsEIC"): get rtrange slot

sampnames signature(object = "xcmsEIC"): get sample names

Note

No notes yet.

Author(s)

Colin A. Smith, <csmith@scripps.edu>

See Also

getEIC

---

xcmsFileSource-class *Base class for loading raw data from a file*

Description

Data sources which read data from a file should inherit from this class. The xcms package provides classes to read from netCDF, mzData, mzXML, and mzML files using xcmsFileSource.

This class should be considered virtual and will not work if passed to loadRaw-methods. The reason it is not explicitly virtual is that there does not appear to be a way for a class to be both virtual and have a data part (which lets functions treat objects as if they were character strings).

This class validates that a file exists at the path given.

Objects from the Class

xcmsFileSource objects should not be instantiated directly. Instead, create subclasses and instantiate those.

Slots

.Data: Object of class "character". File path of a file from which to read raw data as the object's data part

Extends

Class "character", from data part. Class "xcmsSource", directly.

Methods

xcmsSource signature(object = "character"): Create an xcmsFileSource object referencing the given file name.

Author(s)

Daniel Hackney <dan@haxney.org>

See Also

xcmsSource

`xcmsFragments` *Constructor for xcmsFragments objects which holds Tandem MS peaks*

Description

EXPERIMANTAL FEATURE

xcmsFragments is an object similar to xcmsSet, which holds peaks picked (or collected) from one or several xcmsRaw objects.

There are still discussions going on about the exact API for MS^n data, so this is likely to change in the future. The code is not yet pipeline-ified.

Usage

```
xcmsFragments(xs, ...)
```

Arguments

`xs`	A `xcmsSet-class` object which contains picked ms1-peaks from one or several experiments
`...`	further arguments to the `collect` method

Details

After running collect(xFragments,xSet) The peaktable of the xcmsFragments includes the ms1Peaks from all experinemts stored in a xcmsSet-object. Further it contains the relevant MSn-peaks from the xcmsRaw-objects, which were created temporarily with the paths in xcmsSet.

Value

An `xcmsFragments` object.

Author(s)

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

See Also

`xcmsFragments-class`, `collect`

`xcmsFragments-class` *Class xcmsFragments, a class for handling Tandem MS and MS^n data*

Description

This class is similar to `xcmsSet` because it stores peaks from a number of individual files. However, xcmsFragments keeps Tandem MS and e.g. Ion Trap or Orbitrap MS^n peaks, including the parent ion relationships.

Objects from the Class

Objects can be created with the `xcmsFragments` constructor and filled with peaks using the collect method.

Slots

`peaks`**:** matrix with colmns peakID (MS1 parent in corresponding xcmsSet), MSnParentPeakID (parent peak within this xcmsFragments), msLevel (e.g. 2 for Tandem MS), rt (retention time in case of LC data), mz (fragment mass-to-charge), intensity (peak intensity extracted from the original `xcmsSet`), sample (the index of the rawData-file).

`MS2spec`**:** This is a list of matrixes. Each matrix in the list is a single collected spectra from `collect`. The column ID's are mz, intensity, and full width half maximum(fwhm). The fwhm column is only relevant if the spectra came from profile data.

`specinfo`**:** This is a matrix with reference data for the spectra in MS2spec. The column id's are preMZ, AccMZ, rtmin, rtmax, ref, CollisionEnergy. The preMZ is precursor mass from the MS1 scan. This mass is given by the XML file. With some instruments this mass is only given as nominal mass, therefore a AccMZ is given which is a weighted average mass from the MS1 scan of the collected spectra. The retention time is given by rtmin and rtmax. The ref column is a pointer to the MS2spec matrix spectra. The collisionEnergy column is the collision Energy for the spectra.

Methods

collect `signature(object = "xcmsFragments")`: gets a xcmsSet-object, collects ms1-peaks from it and the msn-peaks from the corresponding xcmsRaw-files.

plotTree `signature(object = "xcmsFragments")`: prints a (text based) pseudo-tree of the peak-table to display the dependencies of the peaks among each other.

show `signature(object = "xcmsFragments")`: print a human-readable description of this object to the console.

Note

No notes yet.

Author(s)

S. Neumann, J. Kutzera

References

A parallel effort in metabolite profiling data sharing: http://metlin.scripps.edu/

See Also

xcmsRaw

XCMSnExp-class *Data container storing xcms preprocessing results*

Description

The XCMSnExp object is designed to contain all results from metabolomics data preprocessing (chromatographic peak detection, peak grouping (correspondence) and retention time correction). The corresponding elements in the msFeatureData slot are "chromPeaks" (a matrix), "featureDefinitions" (a DataFrame) and "adjustedRtime" (a list of numeric vectors). Note that these should not be accessed directly but rather *via* their accessor methods.

Along with the results, the object contains the processing history that allows to track each processing step along with the used settings. This can be extracted with the processHistory method.

The XCMSnExp object directly extends the OnDiskMSnExp object and provides thus an easy access to the full raw data at any stage of an analysis.

Objects from this class should not be created directly, they are returned as result from the findChromPeaks method.

XCMSnExp objects can be coerced into xcmsSet objects using the as method.

processHistoryTypes returns the available *types* of process histories. These can be passed with argument type to the processHistory method to extract specific process step(s).

profMat: creates a *profile matrix*, which is a n x m matrix, n (rows) representing equally spaced m/z values (bins) and m (columns) the retention time of the corresponding scans. Each cell contains the maximum intensity measured for the specific scan and m/z values. See profMat for more details and description of the various binning methods.

hasAdjustedRtime: whether the object provides adjusted retention times.

hasFeatures: whether the object contains correspondence results (i.e. features).

hasChromPeaks: whether the object contains peak detection results.

adjustedRtime,adjustedRtime<-: extract/set adjusted retention times. adjustedRtime<- should not be called manually, it is called internally by the adjustRtime methods. For XCMSnExp objects, adjustedRtime<- does also apply retention time adjustments to eventually present chromatographic peaks. The bySample parameter allows to specify whether the adjusted retention time should be grouped by sample (file).

featureDefinitions, featureDefinitions<-: extract or set the correspondence results, i.e. the mz-rt features (peak groups). Similar to the chromPeaks it is possible to extract features for specified m/z and/or rt ranges (see chromPeaks for more details).

chromPeaks, chromPeaks<-: extract or set the matrix containing the information on identified chromatographic peaks. Parameter bySample allows to specify whether peaks should be returned ungrouped (default bySample = FALSE) or grouped by sample (bySample = TRUE). The chromPeaks<- method for XCMSnExp objects removes also all correspondence (peak grouping) and retention time correction (alignment) results. The optional arguments rt, mz and ppm allow to extract only chromatographic peaks overlapping (if type = "any") or completely within (if type = "within")

the defined retention time and mz ranges. See description of the return value for details on the returned matrix. Users usually don't have to use the chromPeaks<- method directly as detected chromatographic peaks are added to the object by the findChromPeaks method.

rtime: extracts the retention time for each scan. The bySample parameter allows to return the values grouped by sample/file and adjusted whether adjusted or raw retention times should be returned. By default the method returns adjusted retention times, if they are available (i.e. if retention times were adjusted using the adjustRtime method).

mz: extracts the mz values from each scan of all files within an XCMSnExp object. These values are extracted from the original data files and eventual processing steps are applied *on the fly*. Using the bySample parameter it is possible to switch from the default grouping of mz values by spectrum/scan to a grouping by sample/file.

intensity: extracts the intensity values from each scan of all files within an XCMSnExp object. These values are extracted from the original data files and eventual processing steps are applied *on the fly*. Using the bySample parameter it is possible to switch from the default grouping of intensity values by spectrum/scan to a grouping by sample/file.

spectra: extracts the Spectrum objects containing all data from object. The values are extracted from the original data files and eventual processing steps are applied *on the fly*. By setting bySample = TRUE, the spectra are returned grouped by sample/file. If the XCMSnExp object contains adjusted retention times, these are returned by default in the Spectrum objects (can be overwritten by setting adjusted = FALSE).

processHistory: returns a list with ProcessHistory objects (or objects inheriting from this base class) representing the individual processing steps that have been performed, eventually along with their settings (Param parameter class). Optional arguments fileIndex, type and msLevel allow to restrict to process steps of a certain type or performed on a certain file or MS level.

dropChromPeaks: drops any identified chromatographic peaks and returns the object without that information. Note that for XCMSnExp objects the method drops by default also results from a correspondence (peak grouping) analysis. Adjusted retention times are removed if the alignment has been performed *after* peak detection. This can be overruled with keepAdjustedRtime = TRUE.

dropFeatureDefinitions: drops the results from a correspondence (peak grouping) analysis, i.e. the definition of the mz-rt features and returns the object without that information. Note that for XCMSnExp objects the method will also by default drop retention time adjustment results, if these were performed after the last peak grouping (i.e. which base on the results from the peak grouping that are going to be removed). All related process history steps are removed too as well as eventually filled in peaks (by fillChromPeaks). The parameter keepAdjustedRtime can be used to avoid removal of adjusted retention times.

dropAdjustedRtime: drops any retention time adjustment information and returns the object without adjusted retention time. For XCMSnExp objects, this also reverts the retention times reported for the chromatographic peaks in the peak matrix to the original, raw, ones (after chromatographic peak detection). Note that for XCMSnExp objects the method drops also all peak grouping results if these were performed *after* the retention time adjustment. All related process history steps are removed too.

findChromPeaks performs chromatographic peak detection on the provided XCMSnExp objects. For more details see the method for XCMSnExp. Note that the findChromPeaks method for XCMSnExp objects removes previously identified chromatographic peaks and aligned features. Previous alignment (retention time adjustment) results are kept, i.e. chromatographic peak detection is performed using adjusted retention times if the data was first aligned using e.g. obiwarp (adjustRtime-obiwarp).

dropFilledChromPeaks: drops any filled-in chromatographic peaks (filled in by the fillChromPeaks method) and all related process history steps.

description spectrapply applies the provided function to each Spectrum in the object and returns its results. If no function is specified the function simply returns the list of Spectrum objects.

Usage

```
processHistoryTypes()

## S4 method for signature 'OnDiskMSnExp'
profMat(object, method = "bin", step = 0.1,
  baselevel = NULL, basespace = NULL, mzrange. = NULL, fileIndex, ...)

## S4 method for signature 'XCMSnExp'
show(object)

## S4 method for signature 'XCMSnExp'
hasAdjustedRtime(object)

## S4 method for signature 'XCMSnExp'
hasFeatures(object)

## S4 method for signature 'XCMSnExp'
hasChromPeaks(object)

## S4 method for signature 'XCMSnExp'
adjustedRtime(object, bySample = FALSE)

## S4 replacement method for signature 'XCMSnExp'
adjustedRtime(object) <- value

## S4 method for signature 'XCMSnExp'
featureDefinitions(object, mz = numeric(),
  rt = numeric(), ppm = 0, type = "any")

## S4 replacement method for signature 'XCMSnExp'
featureDefinitions(object) <- value

## S4 method for signature 'XCMSnExp'
chromPeaks(object, bySample = FALSE, rt = numeric(),
  mz = numeric(), ppm = 0, type = "any")

## S4 replacement method for signature 'XCMSnExp'
chromPeaks(object) <- value

## S4 method for signature 'XCMSnExp'
rtime(object, bySample = FALSE,
  adjusted = hasAdjustedRtime(object))

## S4 method for signature 'XCMSnExp'
mz(object, bySample = FALSE, BPPARAM = bpparam())

## S4 method for signature 'XCMSnExp'
intensity(object, bySample = FALSE,
  BPPARAM = bpparam())

## S4 method for signature 'XCMSnExp'
spectra(object, bySample = FALSE,
```

```
  adjusted = hasAdjustedRtime(object), BPPARAM = bpparam())

## S4 method for signature 'XCMSnExp'
processHistory(object, fileIndex, type, msLevel)

## S4 method for signature 'XCMSnExp'
dropChromPeaks(object, keepAdjustedRtime = FALSE)

## S4 method for signature 'XCMSnExp'
dropFeatureDefinitions(object, keepAdjustedRtime = FALSE,
  dropLastN = -1)

## S4 method for signature 'XCMSnExp'
dropAdjustedRtime(object)

## S4 method for signature 'XCMSnExp'
profMat(object, method = "bin", step = 0.1,
  baselevel = NULL, basespace = NULL, mzrange. = NULL, fileIndex, ...)

## S4 method for signature 'XCMSnExp,Param'
findChromPeaks(object, param, BPPARAM = bpparam(),
  return.type = "XCMSnExp", msLevel = 1L)

## S4 method for signature 'XCMSnExp'
dropFilledChromPeaks(object)

## S4 method for signature 'XCMSnExp'
spectrapply(object, FUN = NULL, BPPARAM = bpparam(),
  ...)
```

Arguments

object	For adjustedRtime, featureDefinitions, chromPeaks, hasAdjustedRtime, hasFeatures and hasChromPeaks either a MsFeatureData or a XCMSnExp object, for all other methods a XCMSnExp object.
method	The profile matrix generation method. Allowed are "bin", "binlin", "binlinbase" and "intlin". See details section for more information.
step	numeric(1) representing the m/z bin size.
baselevel	numeric(1) representing the base value to which empty elements (i.e. m/z bins without a measured intensity) should be set. Only considered if method = "binlinbase". See baseValue parameter of imputeLinInterpol for more details.
basespace	numeric(1) representing the m/z length after which the signal will drop to the base level. Linear interpolation will be used between consecutive data points falling within 2 * basespace to each other. Only considered if method = "binlinbase". If not specified, it defaults to 0.075. Internally this parameter is translated into the distance parameter of the imputeLinInterpol function by distance = floor(basespace / s See distance parameter of imputeLinInterpol for more details.
mzrange.	Optional numeric(2) manually specifying the mz value range to be used for binnind. If not provided, the whole mz value range is used.
fileIndex	For processHistory: optional numeric specifying the index of the files/samples for which the ProcessHistory objects should be retrieved.

...	Additional parameters.
bySample	logical(1) specifying whether results should be grouped by sample.
value	For adjustedRtime<-: a list (length equal to the number of samples) with numeric vectors representing the adjusted retention times per scan. For featureDefinitions<-: a DataFrame with peak grouping information. See return value for the featureDefinitions method for the expected format. For chromPeaks<-: a matrix with information on detected peaks. See return value for the chromPeaks method for the expected format.
mz	optional numeric(2) defining the mz range for which chromatographic peaks should be returned.
rt	optional numeric(2) defining the retention time range for which chromatographic peaks should be returned.
ppm	optional numeric(1) specifying the ppm by which the mz range should be extended. For a value of ppm = 10, all peaks within mz[1] - ppm / 1e6 and mz[2] + ppm / 1e6 are returned.
type	For processHistory: restrict returned ProcessHistory objects to analysis steps of a certain type. Use the processHistoryTypes to list all supported values. For chromPeaks: character specifying which peaks to return if rt or mz are defined. For type = "any" all chromatographic peaks that *overlap* the range defined by the mz or by the rt. For type = "within" only peaks completely within the range(s) are returned.
adjusted	logical(1) whether adjusted or raw (i.e. the original retention times reported in the files) should be returned.
BPPARAM	Parameter class for parallel processing. See bpparam.
msLevel	integer(1) defining the MS level on which the peak detection should be performed. Defaults to msLevel = 1.
keepAdjustedRtime	For dropFeatureDefinitions,XCMSnExp: logical(1) defining whether eventually present retention time adjustment should not be dropped. By default dropping feature definitions drops retention time adjustment results too.
dropLastN	For dropFeatureDefinitions,XCMSnExp: numeric(1) defining the number of peak grouping related process history steps to remove. By default dropLastN = -1, dropping the chromatographic peaks removes all process history steps related to peak grouping. Setting e.g. dropLastN = 1 will only remove the most recent peak grouping related process history step.
param	A CentWaveParam, MatchedFilterParam, MassifquantParam, MSWParam or CentWavePredIsoParam object with the settings for the chromatographic peak detection algorithm.
return.type	Character specifying what type of object the method should return. Can be either "XCMSnExp" (default), "list" or "xcmsSet".
FUN	For spectrapply: a function that should be applied to each spectrum in the object.

Value

For profMat: a list with a the profile matrix matrix (or matrices if fileIndex was not specified or if length(fileIndex) > 1). See profile-matrix for general help and information about the profile matrix.

For adjustedRtime: if bySample = FALSE a numeric vector with the adjusted retention for each spectrum of all files/samples within the object. If bySample = TRUE a list (length equal to the number of samples) with adjusted retention times grouped by sample. Returns NULL if no adjusted retention times are present.

For featureDefinitions: a DataFrame with peak grouping information, each row corresponding to one mz-rt feature (grouped peaks within and across samples) and columns "mzmed" (median mz value), "mzmin" (minimal mz value), "mzmax" (maximum mz value), "rtmed" (median retention time), "rtmin" (minimal retention time), "rtmax" (maximal retention time) and "peakidx". Column "peakidx" contains a list with indices of chromatographic peaks (rows) in the matrix returned by the chromPeaks method that belong to that feature group. The method returns NULL if no feature definitions are present.

For chromPeaks: if bySample = FALSE a matrix with at least the following columns: "mz" (intensity-weighted mean of mz values of the peak across scans/retention times), "mzmin" (minimal mz value), "mzmax" (maximal mz value), "rt" (retention time for the peak apex), "rtmin" (minimal retention time), "rtmax" (maximal retention time), "into" (integrated, original, intensity of the peak), "maxo" (maximum intentity of the peak), "sample" (sample index in which the peak was identified) and "is_filled" defining whether the chromatographic peak was identified by the peak picking algorithm (0) or was added by the fillChromPeaks method (1). Depending on the employed peak detection algorithm and the verboseColumns parameter of it additional columns might be returned. For bySample = TRUE the chronatographic peaks are returned as a list of matrices, each containing the chromatographic peaks of a specific sample. For samples in which no peaks were detected a matrix with 0 rows is returned.

For rtime: if bySample = FALSE a numeric vector with the retention times of each scan, if bySample = TRUE a list of numeric vectors with the retention times per sample.

For mz: if bySample = FALSE a list with the mz values (numeric vectors) of each scan. If bySample = TRUE a list with the mz values per sample.

For intensity: if bySample = FALSE a list with the intensity values (numeric vectors) of each scan. If bySample = TRUE a list with the intensity values per sample.

For spectra: if bySample = FALSE a list with Spectrum objects. If bySample = TRUE the result is grouped by sample, i.e. as a list of lists, each element in the *outer* list being the list of spectra of the specific file.

For processHistory: a list of ProcessHistory objects providing the details of the individual data processing steps that have been performed.

Slots

.processHistory list with XProcessHistory objects tracking all individual analysis steps that have been performed.

msFeatureData MsFeatureData class extending environment and containing the results from a chromatographic peak detection (element "chromPeaks"), peak grouping (element "featureDefinitions") and retention time correction (element "adjustedRtime") steps. This object should not be manipulated directly.

Note

The "chromPeaks" element in the msFeatureData slot is equivalent to the @peaks slot of the xcmsSet object, the "featureDefinitions" contains information from the @groups and @groupidx slots from an xcmsSet object.

Author(s)

Johannes Rainer

See Also

xcmsSet for the old implementation. OnDiskMSnExp, MSnExp and pSet for a complete list of inherited methods.

findChromPeaks for available peak detection methods returning a XCMSnExp object as a result.

groupChromPeaks for available peak grouping methods and featureDefinitions for the method to extract the feature definitions representing the peak grouping results. adjustRtime for retention time adjustment methods.

chromatogram to extract MS data as Chromatogram objects.

extractMsData for the method to extract MS data as data.frames.

fillChromPeaks for the method to fill-in eventually missing chromatographic peaks for a feature in some samples.

Examples

```
## Loading the data from 2 files of the faahKO package.
library(faahKO)
od <- readMSData(c(system.file("cdf/KO/ko15.CDF", package = "faahKO"),
                   system.file("cdf/KO/ko16.CDF", package = "faahKO")),
                 mode = "onDisk")
## Now we perform a chromatographic peak detection on this data set using the
## matched filter method. We are tuning the settings such that it performs
## faster.
mfp <- MatchedFilterParam(binSize = 6)
xod <- findChromPeaks(od, param = mfp)

## The results from the peak detection are now stored in the XCMSnExp
## object
xod

## The detected peaks can be accessed with the chromPeaks method.
head(chromPeaks(xod))

## The settings of the chromatographic peak detection can be accessed with
## the processHistory method
processHistory(xod)

## Also the parameter class for the peak detection can be accessed
processParam(processHistory(xod)[[1]])

## The XCMSnExp inherits all methods from the pSet and OnDiskMSnExp classes
## defined in Bioconductor's MSnbase package. To access the (raw) retention
## time for each spectrum we can use the rtime method. Setting bySample = TRUE
## would cause the retention times to be grouped by sample
head(rtime(xod))

## Similarly it is possible to extract the mz values or the intensity values
## using the mz and intensity method, respectively, also with the option to
## return the results grouped by sample instead of the default, which is
## grouped by spectrum. Finally, to extract all of the data we can use the
```

```
## spectra method which returns Spectrum objects containing all raw data.
## Note that all these methods read the information from the original input
## files and subsequently apply eventual data processing steps to them.
mzs <- mz(xod, bySample = TRUE)
length(mzs)
lengths(mzs)

## The full data could also be read using the spectra data, which returns
## a list of Spectrum object containing the mz, intensity and rt values.
## spctr <- spectra(xod)
## To get all spectra of the first file we can split them by file
## head(split(spctr, fromFile(xod))[[1]])

############
## Filtering
##
## XCMSnExp objects can be filtered by file, retention time, mz values or
## MS level. For some of these filter preprocessing results (mostly
## retention time correction and peak grouping results) will be dropped.
## Below we filter the XCMSnExp object by file to extract the results for
## only the second file.
xod_2 <- filterFile(xod, file = 2)
xod_2

## Now the objects contains only the idenfified peaks for the second file
head(chromPeaks(xod_2))

head(chromPeaks(xod)[chromPeaks(xod)[, "sample"] == 2, ])

##########
## Coercing to an xcmsSet object
##
## We can also coerce the XCMSnExp object into an xcmsSet object:
xs <- as(xod, "xcmsSet")
head(peaks(xs))
```

`xcmsPapply` Deprecated*: xcmsPapply*

Description

This function is deprecated, use `bplapply` instead.

An apply-like function which uses Rmpi to distribute the processing evenly across a cluster. Will use a non-MPI version if distributed processing is not available.

Usage

```
xcmsPapply(arg_sets, papply_action, papply_commondata = list(),
       show_errors = TRUE, do_trace = FALSE, also_trace = c())
```

Arguments

`arg_sets`	a list, where each item will be given as an argument to papply_action

papply_action	A function which takes one argument. It will be called on each element of arg_sets
papply_commondata	A list containing the names and values of variables to be accessible to the papply_action. 'attach' is used locally to import this list.
show_errors	If set to TRUE, overrides Rmpi's default, and messages for errors which occur in R slaves are produced.
do_trace	If set to TRUE, causes the papply_action function to be traced. i.e. Each statement is output before it is executed by the slaves.
also_trace	If supplied an array of function names, as strings, tracing will also occur for the specified functions.

Details

Similar to apply and lapply, applies a function to all items of a list, and returns a list with the corresponding results.

Uses Rmpi to implement a pull idiom in order to distribute the processing evenly across a cluster. If Rmpi is not available, or there are no slaves, implements this as a non-parallel algorithm.

`xcmsPapply` is a modified version of the papply function from package papply 0.2 (Duane Currie). Parts of the slave function were wrapped in try() to make it failsafe and progress output was added.

Make sure `Rmpi` was installed properly by executing the example below. `Rmpi` was tested with

- OpenMPI : Unix, http://www.open-mpi.org/, don't forget to export `MPI_ROOT` before installing Rmpi e.g. `export MPI_ROOT=/usr/lib/openmpi`
- DeinoMPI : Windows, http://mpi.deino.net/, also see http://www.stats.uwo.ca/faculty/yu/Rmpi/

Value

A list of return values from papply_action. Each value corresponds to the element of arg_sets used as a parameter to papply_action

Note

Does not support distributing recursive calls in parallel. If papply is used inside papply_action, it will call a non-parallel version

Author(s)

Duane Currie <duane.currie@acadiau.ca>, modified by Ralf Tautenhahn <rtautenh@ipb-halle.de>.

References

http://ace.acadiau.ca/math/ACMMaC/software/papply/

Examples

```
## Not run:
library(Rmpi)
library(xcms)

number_lists <- list(1:10,4:40,2:27)
```

```
mpi.spawn.Rslaves(nslaves=2)

results <- xcmsPapply(number_lists,sum)
results

mpi.close.Rslaves()


## End(Not run)
```

---

xcmsPeaks-class *A matrix of peaks*

Description

A matrix of peak information. The actual columns depend on how it is generated (i.e. the findPeaks method).

Objects from the Class

Objects can be created by calls of the form new("xcmsPeaks", ...).

Slots

.Data: The matrix holding the peak information

Extends

Class "matrix", from data part. Class "array", by class "matrix", distance 2. Class "structure", by class "matrix", distance 3. Class "vector", by class "matrix", distance 4, with explicit coerce.

Methods

None yet. Some utilities for working with peak data would be nice.

Author(s)

Michael Lawrence

See Also

findPeaks for detecting peaks in an xcmsRaw.

xcmsRaw *Constructor for xcmsRaw objects which reads NetCDF/mzXML files*

Description

This function handles the task of reading a NetCDF/mzXML file containing LC/MS or GC/MS data into a new xcmsRaw object. It also transforms the data into profile (maxrix) mode for efficient plotting and data exploration.

Usage

```
xcmsRaw(filename, profstep = 1, profmethod = "bin", profparam =
list(), includeMSn=FALSE, mslevel=NULL, scanrange=NULL)

deepCopy(object)
```

Arguments

filename	path name of the NetCDF or mzXML file to read
profstep	step size (in m/z) to use for profile generation
profmethod	method to use for profile generation. See profile-matrix for details and supported values.
profparam	extra parameters to use for profile generation
includeMSn	only for XML file formats: also read MS^n (Tandem-MS of Ion-/Orbi- Trap spectra)
mslevel	move data from mslevel into normal MS1 slots, e.g. for peak picking and visualisation
scanrange	scan range to read
object	An xcmsRaw object

Details

See profile-matrix for details on profile matrix generation methods and settings.

The scanrange to import can be restricted, otherwise all MS1 data is read. If profstep is set to 0, no profile matrix is generated. Unless includeMSn = TRUE only first level MS data is read, not MS/MS, etc.

deepCopy(xraw) will create a copy of the xcmsRaw object with its own copy of mz and intensity data in xraw@env.

Value

A xcmsRaw object.

Author(s)

Colin A. Smith, <csmith@scripps.edu>

References

NetCDF file format: http://my.unidata.ucar.edu/content/software/netcdf/ http://www.astm.org/Standards/E2077.htm http://www.astm.org/Standards/E2078.htm

mzXML file format: http://sashimi.sourceforge.net/software_glossolalia.html

PSI-MS working group who developed mzData and mzML file formats: http://www.psidev.info/index.php?q=node/80

Parser used for XML file formats: http://tools.proteomecenter.org/wiki/index.php?title=Software:RAMP

See Also

xcmsRaw-class, profStep, profMethod xcmsFragments

Examples

```
## Not run:
library(xcms)
library(faahKO)
cdfpath <- system.file("cdf", package = "faahKO")
cdffiles <- list.files(cdfpath, recursive = TRUE, full.names = TRUE)
xr<-xcmsRaw(cdffiles[1])
xr
##This gives some information about the file
names(attributes(xr))
## Lets have a look at the structure of the object

str(xr)
##same but with a preview of each slot in the object
##SO... lets have a look at how this works
head(xr@scanindex)
#[1]    0  429  860 1291 1718 2140
xr@env$mz[425:430]
#[1] 596.3 597.0 597.3 598.1 599.3 200.1
##We can see that the 429 index is the last mz of scan 1 therefore...

mz.scan1<-xr@env$mz[(1+xr@scanindex[1]):xr@scanindex[2]]
intensity.scan1<-xr@env$intensity[(1+xr@scanindex[1]):xr@scanindex[2]]
plot(mz.scan1, intensity.scan1, type="h", main=paste("Scan 1 of file", basename(cdffiles[1]), sep=""))
##the easier way :p
scan1<-getScan(xr, 1)
head(scan1)
plotScan(xr, 1)

## End(Not run)
```

---

xcmsRaw-class *Class xcmsRaw, a class for handling raw data*

Description

This class handles processing and visualization of the raw data from a single LC/MS or GS/MS run. It includes methods for producing a standard suite of plots including individual spectra, multi-scan average spectra, TIC, and EIC. It will also produce a feature list of significant peaks using matched filtration.

Objects from the Class

Objects can be created with the `xcmsRaw` constructor which reads data from a NetCDF file into a new object.

Slots

`acquisitionNum`: Numeric representing the acquisition number of the individual scans/spectra. Length of `acquisitionNum` is equal to the number of spectra/scans in the object and hence equal to the `scantime` slot. Note however that this information is only available in mzML files.

`env`: environment with three variables: `mz` - concatenated m/z values for all scans, `intensity` - corresponding signal intensity for each m/z value, and `profile` - matrix represention of the intensity values with columns representing scans and rows representing equally spaced m/z values. The profile matrix should be extracted with the `profMat` method.

`filepath`: Path to the raw data file

`gradient`: matrix with first row, `time`, containing the time point for interpolation and successive columns representing solvent fractions at each point

`msnAcquisitionNum`: for each scan a unique acquisition number as reported via "spectrum id" (mzData) or "<scan num=...>" and "<scanOrigin num=...>" (mzXML)

`msnCollisionEnergy`: "CollisionEnergy" (mzData) or "collisionEnergy" (mzXML)

`msnLevel`: for each scan the "msLevel" (both mzData and mzXML)

`msnPrecursorCharge`: "ChargeState" (mzData) and "precursorCharge" (mzXML)

`msnPrecursorIntensity`: "Intensity" (mzData) or "precursorIntensity" (mzXML)

`msnPrecursorMz`: "MassToChargeRatio" (mzData) or "precursorMz" (mzXML)

`msnPrecursorScan`: "spectrumRef" (both mzData and mzXML)

`msnRt`: Retention time of the scan

`msnScanindex`: msnScanindex

`mzrange`: numeric vector of length 2 with minimum and maximum m/z values represented in the profile matrix

`polarity`: polarity

`profmethod`: characer value with name of method used for generating the profile matrix.

`profparam`: list to store additional profile matrix generation settings. Use the `profinfo` method to extract all profile matrix creation relevant information.

`scanindex`: integer vector with starting positions of each scan in the `mz` and `intensity` variables (note that index values are based off a 0 initial position instead of 1).

`scantime`: numeric vector with acquisition time (in seconds) for each scan.

`tic`: numeric vector with total ion count (intensity) for each scan

`mslevel`: Numeric representing the MS level that is present in MS1 slot. This slot should be accessed through its getter method `mslevel`.

scanrange: Numeric of length 2 specifying the scan range (or NULL for the full range). This slot should be accessed through its getter method scanrange. Note that the scanrange will always be 1 to the number of scans within the xcmsRaw object, which does not necessarily have to match to the scan index in the original mzML file (e.g. if the original data was subsetted). The acquisitionNum information can be used to track the original *position* of each scan in the mzML file.

Methods

findPeaks signature(object = "xcmsRaw"): feature detection using matched filtration in the chromatographic time domain

getEIC signature(object = "xcmsRaw"): get extracted ion chromatograms in specified m/z ranges. This will return the total ion chromatogram (TIC) if the m/z range corresponds to the full m/z range (i.e. sum of all signals per retention time across all m/z).

getPeaks signature(object = "xcmsRaw"): get data for peaks in specified m/z and time ranges

getScan signature(object = "xcmsRaw"): get m/z and intensity values for a single mass scan

getSpec signature(object = "xcmsRaw"): get average m/z and intensity values for multiple mass scans

image signature(x = "xcmsRaw"): get data for peaks in specified m/z and time ranges

levelplot Create an image of the raw (profile) data m/z against retention time, with the intensity color coded.

mslevel Getter method for the mslevel slot.

plotChrom signature(object = "xcmsRaw"): plot a chromatogram from profile data

plotRaw signature(object = "xcmsRaw"): plot locations of raw intensity data points

plotScan signature(object = "xcmsRaw"): plot a mass spectrum of an individual scan from the raw data

plotSpec signature(object = "xcmsRaw"): plot a mass spectrum from profile data

plotSurf signature(object = "xcmsRaw"): experimental method for plotting 3D surface of profile data with rgl.

plotTIC signature(object = "xcmsRaw"): plot total ion count chromatogram

profinfo signature(object = "xcmsRaw"): returns a list containing the profile generation method and step (profile m/z step size) and eventual additional parameters to the profile function.

profMedFilt signature(object = "xcmsRaw"): median filter profile data in time and m/z dimensions

profMethod<- signature(object = "xcmsRaw"): change the method of generating the profile matrix

profMethod signature(object = "xcmsRaw"): get the method of generating the profile matrix

profMz signature(object = "xcmsRaw"): get vector of m/z values for each row of the profile matrix

profRange signature(object = "xcmsRaw"): interpret flexible ways of specifying subsets of the profile matrix

profStep<- signature(object = "xcmsRaw"): change the m/z step used for generating the profile matrix

profStep signature(object = "xcmsRaw"): get the m/z step used for generating the profile matrix

revMz `signature(object = "xcmsRaw")`: reverse the order of the data points for each scan

scanrange Getter method for the `scanrange` slot. See slot description above for more information.

sortMz `signature(object = "xcmsRaw")`: sort the data points by increasing m/z for each scan

stitch `signature(object = "xcmsRaw")`: Raw data correction for lock mass calibration gaps.

Note

No notes yet.

Author(s)

Colin A. Smith, <csmith@scripps.edu>, Johannes Rainer <johannes.rainer@eurac.edu>

References

A parallel effort in metabolite profiling data sharing: http://metlin.scripps.edu/

See Also

xcmsRaw, subset-xcmsRaw for subsetting by spectra.

`xcmsSet` *Constructor for xcmsSet objects which finds peaks in NetCDF/mzXML files*

Description

This function handles the construction of xcmsSet objects. It finds peaks in batch mode and pre-sorts files from subdirectories into different classes suitable for grouping.

Usage

```
xcmsSet(files = NULL, snames = NULL, sclass = NULL, phenoData = NULL,
        profmethod = "bin", profparam = list(),
        polarity = NULL, lockMassFreq=FALSE,
mslevel=NULL, nSlaves=0, progressCallback=NULL,
        scanrange = NULL, BPPARAM = bpparam(),
        stopOnError = TRUE, ...)
```

Arguments

`files`	path names of the NetCDF/mzXML files to read
`snames`	sample names. By default the file name without extension is used.
`sclass`	sample classes.
`phenoData`	`data.frame` or `AnnotatedDataFrame` defining the sample names and classes and other sample related properties. If not provided, the argument `sclass` or the subdirectories in which the samples are stored will be used to specify sample grouping.

profmethod	Method to use for profile generation. Supported values are "bin", "binlin", "binlinbase" and "intlin" (for methods profBin, profBinLin, profBinLinBase and profIntLin, respectively). See help on profBin for a complete list of available methods and their supported parameters.
profparam	parameters to use for profile generation.
polarity	filter raw data for positive/negative scans
lockMassFreq	Performs correction for Waters LockMass function
mslevel	perform peak picking on data of given mslevel
nSlaves	*DEPRECATED*, use BPPARAM argument instead.
progressCallback	function to be called, when progressInfo changes (useful for GUIs)
scanrange	scan range to read
BPPARAM	a BiocParallel parameter object to control how and if parallel processing should be performed. Such objects can be created by the SerialParam, MulticoreParam or SnowParam functions.
stopOnError	Logical specifying whether the feature detection call should stop on the first encountered error (the default), or whether feature detection is performed in all files regardless eventual failures for individual files in which case all errors are reported as warnings.
...	further arguments to the findPeaks method of the xcmsRaw class

Details

The default values of the files, snames, sclass, and phenoData arguments cause the function to recursively search for readable files. The filename without extention is used for the sample name. The subdirectory path is used for the sample class. If the files contain both positive and negative spectra, the polarity can be selected explicitly. The default (NULL) is to read all scans.

If phenoData is provided, it is stored to the phenoData slot of the returned xcmsSet class. If that data.frame contains a column named "class", its content will be returned by the sampclass method and thus be used for the group/class assignment of the individual files (e.g. for peak grouping etc.). For more details see the help of the xcmsSet-class.

The step size (in m/z) to use for profile generation can be submitted either using the profparam argument (e.g. profparam=list(step=0.1)) or by submitting step=0.1. By specifying a value of 0 the profile matrix generation can be skipped.

The feature/peak detection algorithm can be specified with the method argument which defaults to the "matchFilter" method (findPeaks.matchedFilter). Possible values are returned by getOption("BioC")$xcms$findPeaks.methods.

The lock mass correction allows for the lock mass scan to be added back in with the last working scan. This correction gives better reproducibility between sample sets.

Value

A xcmsSet object.

Note

The arguments profmethod and profparam have no influence on the feature/peak detection. The step size parameter step for the profile generation in the findPeaks.matchedFilter peak detection algorithm can be passed using the ....

Author(s)

Colin A. Smith, <csmith@scripps.edu>

See Also

xcmsSet-class, findPeaks, profStep, profMethod, profBin, xcmsPapply

---

xcmsSet-class *Class xcmsSet, a class for preprocessing peak data*

Description

This class transforms a set of peaks from multiple LC/MS or GC/MS samples into a matrix of preprocessed data. It groups the peaks and does nonlinear retention time correction without internal standards. It fills in missing peak values from raw data. Lastly, it generates extracted ion chromatograms for ions of interest.

Details

The phenoData slot (and phenoData parameter in the xcmsSet function) is intended to contain a data.frame describing all experimental factors, i.e. the samples along with their properties. If this data.frame contains a column named "class", this will be returned by the sampclass method and will thus be used by all methods to determine the sample grouping/class assignment (e.g. to define the colors in various plots or for the group method).

The sampclass<- method adds or replaces the "class" column in the phenoData slot. If a data.frame is submitted to this method, the interaction of its columns will be stored into the "class" column.

Also, similar to other classes in Bioconductor, the $ method can be used to directly access all columns in the phenoData slot (e.g. use xset$name on a xcmsSet object called "xset" to extract the values from a column named "name" in the phenoData slot).

Objects from the Class

Objects can be created with the xcmsSet constructor which gathers peaks from a set NetCDF files. Objects can also be created by calls of the form new("xcmsSet", ...).

Slots

peaks matrix containing peak data.

filled A vector with peak indices of peaks which have been added by a fillPeaks method.

groups Matrix containing statistics about peak groups.

groupidx List containing indices of peaks in each group.

phenoData A data.frame containing the experimental design factors.

rt list containing two lists, raw and corrected, each containing retention times for every scan of every sample.

filepaths Character vector with absolute path name of each NetCDF file.

profinfo list containing the values method - profile generation method, and step - profile m/z step size and eventual additional parameters to the profile function.

dataCorrection logical vector filled if the waters Lock mass correction parameter is used.

polarity A string ("positive" or "negative" or NULL) describing whether only positive or negative scans have been used reading the raw data.

progressInfo Progress informations for some xcms functions (for GUI).

progressCallback Function to be called, when progressInfo changes (for GUI).

mslevel Numeric representing the MS level on which the peak picking was performed (by default on MS1). This slot should be accessed through its getter method `mslevel`.

scanrange Numeric of length 2 specifying the scan range (or `NULL` for the full range). This slot should be accessed through its getter method `scanrange`. The scan range provided in this slot represents the scans to which the whole raw data is subsetted.

.processHistory Internal slot to be used to keep track of performed processing steps. This slot should not be directly accessed by the user.

Methods

c `signature("xcmsSet")`: combine objects together

filepaths<- `signature(object = "xcmsSet")`: set `filepaths` slot

filepaths `signature(object = "xcmsSet")`: get `filepaths` slot

diffreport `signature(object = "xcmsSet")`: create report of differentially regulated ions including EICs

fillPeaks `signature(object = "xcmsSet")`: fill in peak data for groups with missing peaks

getEIC `signature(object = "xcmsSet")`: get list of EICs for each sample in the set

getXcmsRaw `signature(object = "xcmsSet", sampleidx = 1,profmethod = profMethod(object), profstep` read the raw data for one or more files in the `xcmsSet` and return it. The default parameters will apply all settings used in the original `xcmsSet` call to generate the `xcmsSet` object to be applied also to the raw data. Parameter `sampleidx` allows to specify which raw file(s) should be loaded. Argument `BPPARAM` allows to setup parallel processing.

groupidx<- `signature(object = "xcmsSet")`: set `groupidx` slot

groupidx `signature(object = "xcmsSet")`: get `groupidx` slot

groupnames `signature(object = "xcmsSet")`: get textual names for peak groups

groups<- `signature(object = "xcmsSet")`: set `groups` slot

groups `signature(object = "xcmsSet")`: get `groups` slot

groupval `signature(object = "xcmsSet")`: get matrix of values from peak data with a row for each peak group

group `signature(object = "xcmsSet")`: find groups of peaks across samples that share similar m/z and retention times

mslevel Getter method for the `mslevel` slot.

peaks<- `signature(object = "xcmsSet")`: set `peaks` slot

peaks `signature(object = "xcmsSet")`: get `peaks` slot

plotrt `signature(object = "xcmsSet")`: plot retention time deviation profiles

profinfo<- `signature(object = "xcmsSet")`: set `profinfo` slot

profinfo `signature(object = "xcmsSet")`: get `profinfo` slot

profMethod `signature(object = "xcmsSet")`: extract the method used to generate the profile matrix.

profStep `signature(object = "xcmsSet")`: extract the profile step used for the generation of the profile matrix.

retcor `signature(object = "xcmsSet")`: use initial grouping of peaks to do nonlinear loess retention time correction

sampclass<- `signature(object = "xcmsSet")`: Replaces the column "class" in the `phenoData` slot. See details for more information.

sampclass `signature(object = "xcmsSet")`: Returns the content of the column "class" from the `phenoData` slot or, if not present, the interaction of the experimental design factors (i.e. of the `phenoData` `data.frame`). See details for more information.

phenoData<- `signature(object = "xcmsSet")`: set the `phenoData` slot

phenoData `signature(object = "xcmsSet")`: get the `phenoData` slot

progressCallback<- `signature(object = "xcmsSet")`: set the `progressCallback` slot

progressCallback `signature(object = "xcmsSet")`: get the `progressCallback` slot

scanrange Getter method for the `scanrange` slot. See scanrange slot description above for more details.

sampnames<- `signature(object = "xcmsSet")`: set rownames in the `phenoData` slot

sampnames `signature(object = "xcmsSet")`: get rownames in the `phenoData` slot

split `signature("xcmsSet")`: divide the xcmsSet into a list of xcmsSet objects depending on the provided factor. Note that only peak data will be preserved, i.e. eventual peak grouping information will be lost.

`object$name`, `object$name<-value` Access and set `name` column in `phenoData`

`object[, i]` Conducts subsetting of a `xcmsSet` instance. Only subsetting on columns, i.e. samples, is supported. Subsetting is performed on all slots, also on `groups` and `groupidx`. Parameter `i` can be an integer vector, a logical vector or a character vector of sample names (matching `sampnames`).

Note

No notes yet.

Author(s)

Colin A. Smith, <csmith@scripps.edu>, Johannes Rainer <johannes.rainer@eurac.edu>

References

A parallel effort in metabolite profiling data sharing: http://metlin.scripps.edu/

See Also

`xcmsSet`

xcmsSource-class *Virtual class for raw data sources*

Description

This virtual class provides an implementation-independent way to load mass spectrometer data from various sources for use in an xcmsRaw object. Subclasses can be defined to enable data to be loaded from user-specified sources. The virtual class xcmsFileSource is included out of the box which contains a file name as a character string.

When implementing child classes of xcmsSource, a corresponding loadRaw-methods method must be provided which accepts the xcmsSource child class and returns a list in the format described in loadRaw-methods.

Objects from the Class

A virtual Class: No objects may be created from it.

Author(s)

Daniel Hackney, <dan@haxney.org>

See Also

xcmsSource-methods for creating xcmsSource objects in various ways.

xcmsSource-methods *Create an xcmsSource object in a flexible way*

Description

Users can define alternate means of reading data for xcmsRaw objects by creating new implementations of this method.

Methods

signature(object = "xcmsSource") Pass the object through unmodified.

Author(s)

Daniel Hackney, <dan@haxney.org>

See Also

xcmsSource

`[,XCMSnExp,ANY,ANY,ANY-method`
XCMSnExp filtering and subsetting

Description

The `[` method allows to subset a `XCMSnExp` object by spectra. Be aware that the `[` method removes all preprocessing results, except adjusted retention times if `keepAdjustedRtime = TRUE` is passed to the method.

`[[` extracts a single `Spectrum` object from an `XCMSnExp`. The reported retention time is the adjusted retention time if alignment has been performed on `x`.

`filterMsLevel`: reduces the `XCMSnExp` object to spectra of the specified MS level(s). See `filterMsLevel` documentation for details and examples. Presently, if `msLevel.` is provided, the function removes identified chromatographic peaks and correspondence results while keeping adjusted retention times by default (if present). The latter can be changed setting `keepAdjustedRtime = FALSE`.

The methods listed on this page allow to filter and subset `XCMSnExp` objects. Most of them are inherited from the `OnDiskMSnExp` object and have been adapted for `XCMSnExp` to enable subsetting also on the preprocessing results.

`filterFile`: allows to reduce the `XCMSnExp` to data from only certain files. Identified chromatographic peaks for these files are retained while all eventually present features (peak grouping information) are dropped. By default also adjusted retention times are removed (if present). This can be overwritten by setting `keepAdjustedRtime = TRUE`.

`filterMz`: filters the data set based on the provided mz value range. All chromatographic peaks and features (grouped peaks) falling completely within the provided mz value range are retained (if their minimal mz value is `>= mz[1]` and the maximal mz value `<= mz[2]`. Adjusted retention times, if present, are not altered by the filtering.

`filterRt`: filters the data set based on the provided retention time range. All chromatographic peaks and features (grouped peaks) the specified retention time window are retained (i.e. if the retention time corresponding to the peak's apex is within the specified rt range). If retention time correction has been performed, the method will by default filter the object by adjusted retention times. The argument `adjusted` allows to specify manually whether filtering should be performed by raw or adjusted retention times. Filtering by retention time does not drop any preprocessing results nor does it remove or change alignment results (i.e. adjusted retention times). The method returns an empty object if no spectrum or feature is within the specified retention time range.

`split` splits an `XCMSnExp` object into a `list` of `XCMSnExp` objects based on the provided parameter `f`. Note that by default all pre-processing results are removed by the splitting, except adjusted retention times, if the optional argument `keepAdjustedRtime = TRUE` is provided.

Usage

```
## S4 method for signature 'XCMSnExp,ANY,ANY,ANY'
x[i, j, ..., drop = TRUE]

## S4 method for signature 'XCMSnExp,ANY,ANY'
x[[i, j, drop = FALSE]]

## S4 method for signature 'XCMSnExp'
filterMsLevel(object, msLevel.,
```

```
  keepAdjustedRtime = hasAdjustedRtime(object))

## S4 method for signature 'XCMSnExp'
filterFile(object, file, keepAdjustedRtime = FALSE)

## S4 method for signature 'XCMSnExp'
filterMz(object, mz, msLevel., ...)

## S4 method for signature 'XCMSnExp'
filterRt(object, rt, msLevel.,
  adjusted = hasAdjustedRtime(object))

## S4 method for signature 'XCMSnExp,ANY'
split(x, f, drop = FALSE, ...)
```

Arguments

x	For [and [[: an XCMSnExp object.
i	For [: numeric or logical vector specifying to which spectra the data set should be reduced. For [[: a single integer or character.
j	For [and [[: not supported.
...	Optional additional arguments.
drop	For [and [[: not supported.
object	A XCMSnExp object.
msLevel.	For filterMz, filterRt, numeric(1) defining the MS level(s) to which operations should be applied or to which the object should be subsetted. See filterMz for more details
keepAdjustedRtime	For filterFile, filterMsLevel, [split: logical(1) defining whether the adjusted retention times should be kept, even if e.g. features are being removed (and the retention time correction was performed on these features).
file	For filterFile: integer defining the file index within the object to subset the object by file or character specifying the file names to sub set. The indices are expected to be increasingly ordered, if not they are ordered internally.
mz	For filterMz: numeric(2) defining the lower and upper mz value for the filtering.
rt	For filterRt: numeric(2) defining the retention time window (lower and upper bound) for the filtering.
adjusted	For filterRt: logical indicating whether the object should be filtered by original (adjusted = FALSE) or adjusted retention times (adjusted = TRUE). For spectra: whether the retention times in the individual Spectrum objects should be the adjusted or raw retention times.
f	For split a vector of length equal to the length of x defining how x will be splitted. It is converted internally to a factor.

Details

All subsetting methods try to ensure that the returned data is consistent. Correspondence results for example are removed if the data set is sub-setted by file, since the correspondence results are dependent on the files on which correspondence was performed. Thus, some filter and sub-setting

methods drop some of the preprocessing results. An exception are the adjusted retention times: most subsetting methods support the argument `keepAdjustedRtime` (even the `[` method) that forces the adjusted retention times to be retained even if the default would be to drop them.

Value

All methods return an `XCMSnExp` object.

Note

The `filterFile` method removes also process history steps not related to the files to which the object should be sub-setted and updates the `fileIndex` attribute accordingly. Also, the method does not allow arbitrary ordering of the files or re-ordering of the files within the object.

Note also that most of the filtering methods, and also the subsetting operations `[` drop all or selected preprocessing results. To consolidate the alignment results, i.e. ensure that adjusted retention times are always preserved, use the `applyAdjustedRtime` function on the object that contains the alignment results. This replaces the raw retention times with the adjusted ones.

Author(s)

Johannes Rainer

See Also

`XCMSnExp` for base class documentation.

Examples

```
## Load some of the files from the faahKO package.
library(faahKO)
fs <- c(system.file('cdf/KO/ko15.CDF', package = "faahKO"),
        system.file('cdf/KO/ko16.CDF', package = "faahKO"),
        system.file('cdf/KO/ko18.CDF', package = "faahKO"))
## Read the files
od <- readMSData(fs, mode = "onDisk")

## Perform peak detection on them using the matched filter algorithm. Note
## that we use a large value for binSize to reduce the runtime of the
## example code.
mfp <- MatchedFilterParam(binSize = 5)
xod <- findChromPeaks(od, param = mfp)

## Subset the dataset to the first and third file.
xod_sub <- filterFile(xod, file = c(1, 3))

## The number of chromatographic peaks per file for the full object
table(chromPeaks(xod)[, "sample"])

## The number of chromatographic peaks per file for the subset
table(chromPeaks(xod_sub)[, "sample"])

basename(fileNames(xod))
basename(fileNames(xod_sub))

## Filter on mz values; chromatographic peaks and features within the
```

```
## mz range are retained (as well as adjusted retention times).
xod_sub <- filterMz(xod, mz = c(300, 400))
head(chromPeaks(xod_sub))
nrow(chromPeaks(xod_sub))
nrow(chromPeaks(xod))

## Filter on rt values. All chromatographic peaks and features within the
## retention time range are retained. Filtering is performed by default on
## adjusted retention times, if present.
xod_sub <- filterRt(xod, rt = c(2700, 2900))

range(rtime(xod_sub))
head(chromPeaks(xod_sub))
range(chromPeaks(xod_sub)[, "rt"])

nrow(chromPeaks(xod))
nrow(chromPeaks(xod_sub))

## Extract a single Spectrum
xod[[4]]

## Subsetting using [ removes all preprocessing results - using
## keepAdjustedRtime = TRUE would keep adjusted retention times, if present.
xod_sub <- xod[fromFile(xod) == 1]
xod_sub

## Using split does also remove preprocessing results, but it supports the
## optional parameter keepAdjustedRtime.
## Split the object into a list of XCMSnExp objects, one per file
xod_list <- split(xod, f = fromFile(xod))
xod_list
```

[,xcmsRaw,logicalOrNumeric,missing,missing-method

Subset an xcmsRaw object by scans

Description

Subset an xcmsRaw object by scans. The returned xcmsRaw object contains values for all scans specified with argument i. Note that the scanrange slot of the returned xcmsRaw will be c(1, length(object@scantime)) and hence not range(i).

Usage

```
## S4 method for signature 'xcmsRaw,logicalOrNumeric,missing,missing'
x[i, j, drop]
```

Arguments

x	The xcmsRaw object that should be sub-setted.
i	Integer or logical vector specifying the scans/spectra to which x should be sub-setted.
j	Not supported.
drop	Not supported.

Details

Only subsetting by scan index in increasing order or by a logical vector are supported. If not ordered, argument `i` is sorted automatically. Indices which are larger than the total number of scans are discarded.

Value

The sub-setted `xcmsRaw` object.

Author(s)

Johannes Rainer

See Also

`split.xcmsRaw`

Examples

```
## Load a test file
file <- system.file('cdf/KO/ko15.CDF', package = "faahKO")
xraw <- xcmsRaw(file)
## The number of scans/spectra:
length(xraw@scantime)

## Subset the object to scans with a scan time from 3500 to 4000.
xsub <- xraw[xraw@scantime >= 3500 & xraw@scantime <= 4000]
range(xsub@scantime)
## The number of scans:
length(xsub@scantime)
## The number of values of the subset:
length(xsub@env$mz)
```

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