

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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<https://github.com/sneumann/xcms>

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'cwTools.R' 'databases.R' 'functions-MsFeatureData.R'
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'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-imputation.R' 'functions-normalization.R'
 'functions-xcmsEIC.R' 'functions-xcmsFragments.R'
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 'models.R' 'mzClust.R' 'netCDF.R' 'plotQC.R' 'ramp.R'
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absent-methods	<i>Determine which peaks are absent / present in a sample class</i>
----------------	---

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 alignment 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 <i>profile matrix</i> 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 <code>floor(median(1:length(fileNameNames(object))))</code> .
response	numeric(1) defining the <i>responsiveness</i> of warping with <code>response = 0</code> giving linear warping on start and end points and <code>response = 100</code> 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 <code>distFun = "cor_opt"</code> .
gapInit	numeric(1) defining the penalty for gap opening. The default value for <code>gapInit</code> depends on the value of <code>distFun</code> : for <code>distFun = "cor"</code> and <code>distFun = "cor_opt"</code> it is 0.3, for <code>distFun = "cov"</code> and <code>distFun = "prd"</code> 0.0 and for <code>distFun = "euc"</code> 0.9.
gapExtend	numeric(1) defining the penalty for gap enlargement. The default value for <code>gapExtend</code> depends on the value of <code>distFun</code> , for <code>distFun = "cor"</code> and <code>distFun = "cor_opt"</code> it is 2.4, for <code>distFun = "cov"</code> 11.7, for <code>distFun = "euc"</code> 1.8 and for <code>distFun = "prd"</code> 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 <code>XCMSnExp</code> object. For all other methods: a <code>ObiwrapParam</code> object.
param	A <code>ObiwrapParam</code> 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 `ObiwrapParam` function returns a `ObiwrapParam` class instance with all of the settings specified for `obiwarp` retention time adjustment and alignment.

For `adjustRtime`, `XCMSnExp`, `ObiwrapParam`: 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`, `ObiwrapParam`: 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 `ObiwrapParam` 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 $\leq 6 + 1$. 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 in the MSnbase package for more details and examples.

[clean](#): removes unused 0 intensity data points. See [clean](#) documentation in the MSnbase package 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 in the MSnbase package 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 in MSnbase 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 in the MSnbase package for details. For pickPeaks: character(1) defining the method. See pickPeaks for options. For smooth: character(1) defining the method. See smooth in the MSnbase package 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 in the MSnbase package 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

<i>x</i>	Numeric vector to be used for binning.
<i>y</i>	Numeric vector (same length than <i>x</i>) from which the maximum values for each bin should be defined. If not provided, <i>x</i> will be used.
<i>breaks</i>	Numeric vector defining the breaks for the bins, i.e. the lower and upper values for each bin. See examples below.
<i>nBins</i>	<code>integer(1)</code> defining the number of desired bins.
<i>binSize</i>	<code>numeric(1)</code> defining the desired bin size.
<i>binFromX</i>	Optional <code>numeric(1)</code> allowing to manually specify the range of <i>x</i> -values to be used for binning. This will affect only the calculation of the breaks for the bins (i.e. if <i>nBins</i> or <i>binSize</i> is provided). If not provided the minimal value in the sub-set <code>fromIdx-toIdx</code> in input vector <i>x</i> will be used.
<i>binToX</i>	Same as <i>binFromX</i> , but defining the maximum <i>x</i> -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 $x[\text{fromIdx}]$ to $x[\text{toIdx}]$. 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 = nBins)`. 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 \geq `xlower` and $<$ `xupper` (with `xlower` and `xupper` being the lower and upper boundary, respectively). For the last bin the condition is $x \geq$ `xlower` & $x \leq$ `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 to `X + 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
##  $\geq$  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 on 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 from 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 comparison 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	<i>Generate breaks for binning</i>
-----------------	------------------------------------

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

<code>xs1</code>	<code>xcmsSet</code> object
<code>...</code>	<code>xcmsSet</code> 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 chromatographic 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

<code>mz</code>	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 <code>XCMSnExp</code> object. If a list is provided, it's length has to be equal to the number of samples in the experiment.
<code>mzabs</code>	numeric(1) the absolute error/deviation for matching peaks to calibrants (in Da).
<code>mzppm</code>	numeric(1) the relative error for matching peaks to calibrants in ppm (parts per million).
<code>neighbors</code>	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.
<code>method</code>	character(1) defining the method that should be used to estimate the calibration function. Can be "shift", "linear" (default) or "edgeshift".
<code>object</code>	An <code>XCMSnExp</code> object.
<code>param</code>	The <code>CalibrantMassParam</code> 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 $\leq \text{mzabs} + \text{mz} * \text{mzppm} / 1\text{e}6$.

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

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

<code>object</code>	a <code>xcmsSet</code> object with uncalibrated m/z
<code>calibrants</code>	a vector or a list of vectors with reference m/z-values
<code>method</code>	the used calibrating-method, see below
<code>mzppm</code>	the relative error used for matching peaks in ppm (parts per million)
<code>mzabs</code>	the absolute error used for matching peaks in Da
<code>neighbours</code>	the number of neighbours from which the one with the highest intensity is used (instead of the nearest)
<code>plotres</code>	can be set to <code>TRUE</code> 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,`

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 m/z 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 m/z 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 m/z 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 m/z 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.

[as](#) (`as(x, "data.frame")`) in [MSnbase](#) 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(runtime(chrs[1, 2]), intensity(chrs[1, 2]), type = "l", xlab = "runtime",
     ylab = "intensity", col = "000080")
for(i in c(1, 3)) {
  points(runtime(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](#)

chromPeakSpectra

Extract (MS2) spectra associated with chromatographic peaks

Description

Extract (MS2) spectra from an [XCMSnExp](#) object that represent ions within the rt and m/z range defined by each chromatographic peak (in the same file /sample in which the peak was detected).

Usage

```
chromPeakSpectra(x, msLevel = 2L, expandRt = 0, expandMz = 0,
  ppm = 0, method = c("all", "closest_rt", "closest_mz", "signal"),
  skipFilled = FALSE, return.type = c("Spectra", "list"))
```

Arguments

x	XCMSnExp object with identified chromatographic peaks.
msLevel	integer(1) defining whether MS1 or MS2 spectra should be returned. Currently only msLevel = 2 is supported.
expandRt	numeric(1) to expand the retention time range of each peak by a constant value on each side.
expandMz	numeric(1) to expand the m/z range of each peak by a constant value on each side.
ppm	numeric(1) to expand the m/z range of each peak (on each side) by a value dependent on the peak's m/z.

method	character(1) specifying which MS2 spectra should be included. Defaults to "all" in which all MS2 spectra within the rt and m/z range of a chromatographic peak are returned. "closest_rt" returns the one MS2 spectrum with the retention time closest to the chromatographic peak's apex rt. "closest_mz" returns the MS2 spectrum with the precursor m/z closest to the chromatographic peak's m/z. "signal" returns the MS2 spectrum which total signal is closest to the chromatographic peak's maximal signal ("maxo").
skipFilled	logical(1) whether no spectra for filled-in peaks should be reported.
return.type	character(1) defining whether the result should be a Spectra object or a simple list. See below for more information.

Value

Which object is returned depends on the value of return.type:

- For return.type = "Spectra": a [Spectra](#) object with elements being [Spectrum](#) objects. The result objects contains all spectra that for all peaks. Metadata column "peak_id" provides the ID of the respective peak (i.e. its rowname in [chromPeaks](#)).
- If return.type = "list": list of lists that are either of length 0 or contain [Spectrum2](#) object(s) within the m/z-rt range. The length of the list matches the number of peaks.

Author(s)

Johannes Rainer

collect-methods	<i>Collect MSⁿ peaks into xcmsFragments</i>
-----------------	--

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.
missing	numeric(1) defining an optional value for missing values. missing = 0 would e.g. replace all NA values in the feature matrix with 0. Note that also a call to fillPeaks results in a feature matrix in which NA values are replaced by 0.
...	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 <code>tstat</code> for which set of sample classes was higher)
tstat	Welch's two sample t-statistic, positive for analytes having greater intensity in <code>class2</code> , negative for analytes having greater intensity in <code>class1</code>
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
  numeric(), ...)
```

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) containing 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 be 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 $\leq 6 + 1$. 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 parameters 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, mzdifff = -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.
mzdifff	numeric(1) representing the minimum difference in m/z dimension required for peaks with overlapping retention times; can be negative to allow overlap. During peak post-processing, peaks defined to be overlapping are reduced to the one peak with the largest signal.

fitgauss	logical(1) whether or not a Gaussian should be fitted to each peak. This affects mostly the retention time position of the 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: <code>scmin</code> (start scan index), <code>scmax</code> (end scan index), <code>mzmin</code> (minimum m/z), <code>mzmax</code> (maximum m/z), <code>length</code> (number of scans), <code>intensity</code> (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 <code>roiList</code> defining the scale for each region of interest in <code>roiList</code> that should be used for the <code>centWave</code> -wavelets.
sleep	numeric(1) defining the number of seconds to wait between iterations. Defaults to <code>sleep = 0</code> . 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. In detail, starting with a single m/z, a ROI is extended if a m/z can be found in the next scan (spectrum) for which the difference to the mean m/z of the ROI is smaller than the user defined ppm of the m/z. The mean m/z of the ROI is then updated considering also the newly included m/z value.

These ROIs are then, after some cleanup, 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 $(\text{maxo} - \text{baseline})/\text{sd}$, sd being the standard deviation of local chromatographic noise.

egauss RMSE of Gaussian fit.

Additional columns for `verboseColumns = TRUE`:

mu Gaussian parameter μ .

sigma Gaussian parameter σ .

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 number).

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 Böttcher, 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_massif](#), [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, mzdifff = -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,
  mzdifff = -0.001, fitgauss = FALSE, noise = 0,
  verboseColumns = FALSE, peaks. = NULL, maxCharge = 3, maxIso = 5,
  mzIntervalExtension = TRUE, polarity = "unknown")
```

Arguments

<code>mz</code>	Numeric vector with the individual <code>m/z</code> values from all scans/ spectra of one file/sample.
<code>int</code>	Numeric vector with the individual intensity values from all scans/spectra of one file/sample.
<code>scantime</code>	Numeric vector of length equal to the number of spectra/scans of the data representing the retention time of each scan.
<code>valsPerSpect</code>	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 <i>do_findChromPeaks_addPredIsoROIs</i> : numeric(1) defining the signal to noise threshold for the <i>centWave</i> algorithm. For <i>do_findChromPeaks_centWaveWithPredIsoROIs</i> : numeric(1) defining the signal to noise threshold for the initial (first) <i>centWave</i> 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 $\geq I$.
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 <i>integrate</i> = 1 peak limits are found through descent on the mexican hat filtered data, for <i>integrate</i> = 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 required for peaks with overlapping retention times; can be negative to allow overlap. During peak post-processing, peaks defined to be overlapping are reduced to the one peak with the largest signal.
fitgauss	logical(1) whether or not a Gaussian should be fitted to each peak. This affects mostly the retention time position of the 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: <i>scmin</i> (start scan index), <i>scmax</i> (end scan index), <i>mzmin</i> (minimum m/z), <i>mzmax</i> (maximum m/z), <i>length</i> (number of scans), <i>intensity</i> (summed intensity). Each ROI should be represented by a list of elements or a single row <i>data.frame</i> .
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 <i>roiList</i> defining the scale for each region of interest in <i>roiList</i> that should be used for the <i>centWave</i> -wavelets.
snthreshIsoROIs	numeric(1) defining the signal to noise ratio cutoff to be used in the second <i>centWave</i> 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", "sclmin", "sclmax", "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 $(\text{maxo} - \text{baseline})/\text{sd}$, 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, mzdifff = -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 $\geq I$.
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 required for peaks with overlapping retention times; can be negative to allow overlap. During peak post-processing, peaks defined to be overlapping are reduced to the one peak with the largest signal.
fitgauss	logical(1) whether or not a Gaussian should be fitted to each peak. This affects mostly the retention time position of the 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 prediction 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 the most difficult 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 Minimum 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_centWave](#), [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-derivative Gaussian as the model peak shape. After filtration peaks are detected using a signal-to-ratoin 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,
  mzdifff = 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 required for peaks with overlapping retention times; can be negative to allow overlap. During peak post-processing, peaks defined to be overlapping are reduced to the one peak with the largest signal.
index	logical(1) specifying whether indices 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 $\min(mz) - \text{bin_size}/2$ and $\min(mz) + \text{bin_size}/2$).

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 (\leq 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_centWave](#), [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

<code>mz</code>	Numeric vector with the individual m/z values from all scans/ spectra of one file/sample.
<code>int</code>	Numeric vector with the individual intensity values from all scans/spectra of one file/sample.
<code>snthresh</code>	<code>numeric(1)</code> defining the signal to noise ratio cutoff.
<code>verboseColumns</code>	<code>logical(1)</code> whether additional peak meta data columns should be returned.
<code>...</code>	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_centWave](#), [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 m/z ranges.

Usage

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

Arguments

<code>peaks</code>	A matrix or data.frame with the m/z 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.
<code>sampleGroups</code>	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 <code>PeakDensityParam</code> 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).
<code>bw</code>	numeric(1) defining the bandwidth (standard deviation of the smoothing kernel) to be used. This argument is passed to the <code>density</code> method.
<code>minFraction</code>	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).
<code>minSamples</code>	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).
<code>binSize</code>	numeric(1) defining the size of the overlapping slices in m/z dimension.
<code>maxFeatures</code>	numeric(1) with the maximum number of peak groups to be identified in a single m/z slice.
<code>sleep</code>	numeric(1) defining the time to <i>sleep</i> between iterations and plot the result from the current iteration.

Details

For overlapping slices along the m/z 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

<code>peaks</code>	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.
<code>sampleGroups</code>	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 <code>PeakDensityParam</code> 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).
<code>mzVsRtBalance</code>	numeric(1) representing the factor by which mz values are multiplied before calculating the (euclidian) distance between two peaks.
<code>absMz</code>	numeric(1) maximum tolerated distance for mz values.
<code>absRt</code>	numeric(1) maximum tolerated distance for rt values.
<code>kNN</code>	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>

exportMetaboAnalyst *Export data for use in MetaboAnalyst*

Description

Export the feature table for further analysis in the MetaboAnalyst software (or the MetaboAnalystR R package).

Usage

```
exportMetaboAnalyst(x, file = NULL, label, value = "into",
  digits = NULL, ...)
```

Arguments

x	XCMSnExp object with identified chromatographic peaks grouped across samples.
file	character(1) defining the file name. If not specified, the matrix with the content is returned.
label	either character(1) specifying the phenodata column in x defining the sample grouping or a vector with the same length than samples in x defining the group assignment of the samples.
value	character(1) specifying the value to be returned for each feature. See featureValues() for more details.
digits	integer(1) defining the number of significant digits to be used for numeric. The default NULL uses <code>getOption("digits")</code> . See format() for more information.
...	additional parameters to be passed to the featureValues() function.

Value

If file is not specified, the function returns the matrix in the format supported by MetaboAnalyst.

Author(s)

Johannes Rainer

extractMsData, OnDiskMSnExp-method

DEPRECATED: Extract a data.frame containing MS data

Description

UPDATE: the `extractMsData` and `plotMsData` functions are deprecated and `as(x, "data.frame")` and `plot(x, type = "XIC")` (x being an `OnDiskMSnExp` or `XCMSnExp` object) should be used instead. See examples below. Be aware that filtering the raw object might however drop the adjusted retention times. In such cases it is advisable to use the `applyAdjustedRtime()` function prior to filtering.

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

<code>object</code>	A <code>XCMSnExp</code> or <code>OnDiskMSnExp</code> object.
<code>rt</code>	numeric(2) with the retention time range from which the data should be extracted.
<code>mz</code>	numeric(2) with the mz range.
<code>msLevel</code>	integer defining the MS level(s) to which the data should be sub-setted prior to extraction; defaults to <code>msLevel = 1L</code> .
<code>adjustedRtime</code>	(for <code>extractMsData, XCMSnExp</code>): 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.

Examples

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

## Extract the full data as a data.frame
ms_all <- as(raw_data, "data.frame")
head(ms_all)
nrow(ms_all)

## Read the full MS data for a defined mz-rt region.
res <- raw_data %>%
  filterRt(rt = c(2700, 2900)) %>%
  filterMz(mz = c(300, 320)) %>%
  as("data.frame")

head(res)
nrow(res)
```

featureChromatograms *Extract ion chromatograms for each feature*

Description

Extract ion chromatograms for each feature in an [XCMSnExp](#) object.

Usage

```
featureChromatograms(x, expandRt = 0, aggregationFun = "max", features,
  ...)
```

Arguments

x	XCMSnExp object with grouped chromatographic peaks.
expandRt	numeric(1) to expand the retention time range for each chromatographic peak by a constant value on each side.
aggregationFun	character(1) specifying the name that should be used to aggregate intensity values across the m/z value range for the same retention time. The default "sum" returns a base peak chromatogram.
features	integer, character or logical defining a subset of features for which chromatograms should be returned. Can be the index of the features in featureDefinitions, feature IDs (row names of featureDefinitions) or a logical vector.
...	optional arguments to be passed along to the chromatogram() function.

Value

[Chromatograms](#) object.

Author(s)

Johannes Rainer

Examples

```

library(xcms)
library(faahKO)
faahko_3_files <- c(system.file('cdf/K0/ko15.CDF', package = "faahKO"),
                    system.file('cdf/K0/ko16.CDF', package = "faahKO"),
                    system.file('cdf/K0/ko18.CDF', package = "faahKO"))

## Do a simple and fast preprocessing of the test data
od <- readMSData(faahko_3_files, mode = "onDisk")
od <- findChromPeaks(od, param = CentWaveParam(peakwidth = c(30, 80),
        noise = 1000))
od <- adjustRtime(od, param = ObiwrapParam(binSize = 0.6))
od <- groupChromPeaks(od,
    param = PeakDensityParam(minFraction = 0.8, sampleGroups = rep(1, 3)))

## Extract ion chromatograms for each feature
chrs <- featureChromatograms(od)

## Plot the XIC for the first feature using different colors for each file
par(mfrow = c(1, 2))
plot(chrs[1, ], col = c("red", "green", "blue"))

```

featureSpectra

*Extract (MS2) spectra associated with features***Description**

Return (MS2) spectra for all chromatographic peaks associated with the features in `x` (defined by `featureDefinitions()`).

Usage

```
featureSpectra(x, msLevel = 2, expandRt = 0, expandMz = 0, ppm = 0,
    skipFilled = FALSE, return.type = c("Spectra", "list"), ...)
```

Arguments

<code>x</code>	<code>XCMSnExp</code> object with feature definitions available.
<code>msLevel</code>	integer(1) defining whether MS1 or MS2 spectra should be returned. Currently only <code>msLevel = 2</code> is supported.
<code>expandRt</code>	numeric(1) to expand the retention time range of each peak by a constant value on each side.
<code>expandMz</code>	numeric(1) to expand the m/z range of each peak by a constant value on each side.
<code>ppm</code>	numeric(1) to expand the m/z range of each peak (on each side) by a value dependent on the peak's m/z.

skipFilled	logical(1) whether no spectra for filled-in peaks should be reported.
return.type	character(1) defining whether the result should be a Spectra object or a simple list. See below for more information.
...	additional arguments to be passed along to chromPeakSpectra() , such as method.

Details

The function identifies all MS2 spectra with their precursor m/z within the m/z range of a chromatographic peak of a feature and their retention time within the rt range of the same peak.

The optional parameter method allows to ensure that for each chromatographic peak in one sample only one MS2 spectrum is returned. See [chromPeakSpectra\(\)](#) for more details.

Value

Which object is returned depends on the value of return.type:

- For return.type = "Spectra" (the default): a [Spectra](#) object with data only for features for which a [Spectrum2](#) was found. The ID of the feature and of the chromatographic peak to which the spectrum is associated are provided with the "feature_id" and "peak_id" metadata columns.
- For return.type = "list": a list, same length than there are features in x, each element being a if none are present.

Author(s)

Johannes Rainer

featureSummary	<i>Simple feature summaries</i>
----------------	---------------------------------

Description

Simple function to calculate feature summaries. These include counts and percentages of samples in which a chromatographic peak is present for each feature and counts and percentages of samples in which more than one chromatographic peak was annotated to the feature. Also relative standard deviations (RSD) are calculated for the integrated peak areas per feature across samples. For 'perSampleCounts = TRUE' also the individual chromatographic peak counts per sample are returned.

Usage

```
featureSummary(x, group, perSampleCounts = FALSE, method = "maxint",
  skipFilled = TRUE)
```

Arguments

x	'XCMSnExp' object with correspondence results.
group	'numeric', 'logical', 'character' or 'factor' with the same length than 'x' has samples to aggregate counts by the groups defined in 'group'.
perSampleCounts	'logical(1)' whether feature wise individual peak counts per sample should be returned too.
method	'character' passed to the [featureValues()] function. See respective help page for more information.
skipFilled	'logical(1)' whether filled-in peaks should be excluded (default) or included in the summary calculation.

Value

'matrix' with one row per feature and columns:

- "count": the total number of samples in which a peak was found. - "perc": the percentage of samples in which a peak was found. - "multi_count": the total number of samples in which more than one peak was assigned to the feature. - "multi_perc": the percentage of those samples in which a peak was found, that have also multiple peaks annotated to the feature. Example: for a feature, at least one peak was detected in 50 samples. In 5 of them 2 peaks were assigned to the feature. "multi_perc" is in this case 10 - "rsd": relative standard deviation (coefficient of variation) of the integrated peak area of the feature's peaks. - The same 4 columns are repeated for each unique element (level) in 'group' if 'group' was provided.

If 'perSampleCounts = TRUE' also one column for each sample is returned with the peak counts per sample.

Author(s)

Johannes Rainer

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",
  "sum"), value = "index", intensity = "into", filled = TRUE,
  missing = NA)
```

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 <i>representative</i> 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. If "sum": sum the values (only if value is "into" or "maxo").
value	character specifying the name of the column in <code>chromPeaks(object)</code> that should be returned or "index" (the default) to return the index of the peak in the <code>chromPeaks(object)</code> matrix corresponding to the <i>representative</i> peak for the feature in the respective sample. To return the integrated peak area use <code>value = "into"</code> .
intensity	character specifying the name of the column in the <code>chromPeaks(objects)</code> matrix containing the intensity value of the peak that should be used for the conflict resolution if <code>method = "maxint"</code> .
filled	logical(1) specifying whether values for filled-in peaks should be returned or not. If <code>filled = FALSE</code> , an NA is returned in the matrix for the respective peak. See fillChromPeaks for details on peak filling.
missing	how missing values should be reported. Allowed values are NA (the default), a numeric or <code>missing = "rowmin_half"</code> . The latter replaces any NA with half of the row's minimal (non-missing) value.

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. Note that `missing = 0` should be used to get the same behaviour as `groupval`, i.e. report missing values as 0 after a call to `fillPeaks`.

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,
  fixedMz = 0, fixedRt = 0)
```

```
fixedRt(object)
```

```
fixedMz(object)
```

```
## 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 $\text{expandMz} \times$ 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 peaks with 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 <i>ppm</i> by which the mz width of the peak region should be expanded. For peaks with an mz width smaller than $\text{mean}(c(\text{mzmin}, \text{mzmax})) \times \text{ppm}$, the mzmin will be replaced by $\text{mean}(c(\text{mzmin}, \text{mzmax})) - (\text{mean}(c(\text{mzmin}, \text{mzmax})) \times \text{ppm} / 2 / 1\text{e}6)$ and mzmax by $\text{mean}(c(\text{mzmin}, \text{mzmax})) + (\text{mean}(c(\text{mzmin}, \text{mzmax})) \times \text{ppm} / 2 / 1\text{e}6)$. This is applied before eventually expanding the mz width using the expandMz parameter.
fixedMz	numeric(1) defining a constant factor by which the m/z width of each feature is to be expanded. The m/z width is expanded on both sides by fixedMz (i.e. fixedMz is subtracted from the lower m/z and added to the upper m/z). This expansion is applied <i>after</i> expandMz and ppm.
fixedRt	numeric(1) defining a constant factor by which the retention time width of each factor is to be expanded. The rt width is expanded on both sides by fixedRt (i.e. fixedRt is subtracted from the lower rt and added to the upper rt). This expansion is applied <i>after</i> expandRt.
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. Various parameters allow to increase this area, either by a constant value (`fixedMz` and `fixedRt`) or by a feature-relative amount (`expandMz` and `expandRt`).

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, fixedMz, fixedRt 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(flfs[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(fileName(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 retention 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 thresholded, and the integration area contains no actual raw intensities, or if one sample is miscalibrated, such that 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 proper 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](#)

`filterFeatureDefinitions`*XCMSnExp filtering and subsetting*

Description

`filterFeatureDefinitions` allows to subset the feature definitions of an `XCMSnExp` object. Which feature definitions should be kept can be specified with the `features` argument that can be a logical, integer or character vector. The function returns the `XCMSnExp` with the reduced `featureDefinitions` data frame.

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 \geq `mz[1]` and the maximal `mz` value \leq `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

```
filterFeatureDefinitions(x, features)
```

```
## 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.
features	For filterFeatureDefinitions: either a integer specifying the indices of the features (rows) to keep, a logical with a length matching the number of rows of featureDefinitions or a character with the feature (row) names.
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(fileName(xod))
basename(fileName(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

```

findChromPeaks, Chromatogram, CentWaveParam-method

centWave-based peak detection in purely chromatographic data

Description

findChromPeaks on a [Chromatogram](#) or [Chromatograms](#) object with a [CentWaveParam](#) parameter object performs centWave-based peak detection on purely chromatographic data. See [centWave](#) for details on the method and [CentWaveParam](#) for details on the parameter class. Note that not all settings from the CentWaveParam will be used. See [peaksWithCentWave\(\)](#) for the arguments used for peak detection on purely chromatographic data.

Usage

```
## S4 method for signature 'Chromatogram,CentWaveParam'  
findChromPeaks(object, param, ...)
```

Arguments

object	a Chromatogram or Chromatograms object.
param	a CentWaveParam object specifying the settings for the peak detection. See peaksWithCentWave() for the description of arguments used for peak detection.
...	currently ignored.

Value

If called on a [Chromatogram](#) object, the method returns a matrix with the identified peaks. See [peaksWithCentWave\(\)](#) for details on the matrix content.

Author(s)

Johannes Rainer

See Also

[peaksWithCentWave\(\)](#) for the downstream function and [centWave](#) for details on the method.

Examples

```
od <- readMSData(system.file("cdf/K0/ko15.CDF", package = "faahK0"),  
  mode = "onDisk")  
  
## Extract chromatographic data for a small m/z range  
chr <- chromatogram(od, mz = c(272.1, 272.3))[1, 1]  
  
## Identify peaks with default settings  
pks <- findChromPeaks(chr, CentWaveParam())  
pks  
  
## Plot the identified peaks  
plot(chr, type = "h")  
rect(xleft = pks[, "rtmin"], xright = pks[, "rtmax"],  
  ybottom = rep(0, nrow(pks)), ytop = pks[, "maxo"], col = "#ff000020")  
  
## Modify the settings  
cwp <- CentWaveParam(snthresh = 5, peakwidth = c(10, 60))  
pks <- findChromPeaks(chr, cwp)  
pks  
  
plot(chr, type = "h")  
rect(xleft = pks[, "rtmin"], xright = pks[, "rtmax"],  
  ybottom = rep(0, nrow(pks)), ytop = pks[, "maxo"], col = "#00ff0020")
```

findChromPeaks,Chromatogram,MatchedFilterParam-method

matchedFilter-based peak detection in purely chromatographic data

Description

findChromPeaks on a [Chromatogram](#) or [Chromatograms](#) object with a [MatchedFilterParam](#) parameter object performs matchedFilter-based peak detection on purely chromatographic data. See [matchedFilter](#) for details on the method and [MatchedFilterParam](#) for details on the parameter class. Note that not all settings from the MatchedFilterParam will be used. See [peaksWithMatchedFilter\(\)](#) for the arguments used for peak detection on purely chromatographic data.

Usage

```
## S4 method for signature 'Chromatogram,MatchedFilterParam'  
findChromPeaks(object, param,  
  ...)
```

Arguments

object	a Chromatogram or Chromatograms object.
param	a MatchedFilterParam object specifying the settings for the peak detection. See peaksWithMatchedFilter() for the description of arguments used for peak detection.
...	currently ignored.

Value

If called on a Chromatogram object, the method returns a matrix with the identified peaks. See [peaksWithMatchedFilter\(\)](#) for details on the matrix content.

Author(s)

Johannes Rainer

See Also

[peaksWithMatchedFilter\(\)](#) for the downstream function and [matchedFilter](#) for details on the method.

Examples

```
od <- readMSData(system.file("cdf/KO/ko15.CDF", package = "faahKO"),  
  mode = "onDisk")  
  
## Extract chromatographic data for a small m/z range  
chr <- chromatogram(od, mz = c(272.1, 272.3))[1, 1]  
  
## Identify peaks with default settings  
pks <- findChromPeaks(chr, MatchedFilterParam())  
pks
```



```

## Plot the identified peaks
plot(chr, type = "h")
rect(xleft = pks[, "rtmin"], xright = pks[, "rtmax"],
     ybottom = rep(0, nrow(pks)), ytop = pks[, "maxo"], col = "#ff000020")

## Modify the settings
mfp <- MatchedFilterParam(fwhm = 60)
pks <- findChromPeaks(chr, mfp)
pks

plot(chr, type = "h")
rect(xleft = pks[, "rtmin"], xright = pks[, "rtmax"],
     ybottom = rep(0, nrow(pks)), ytop = pks[, "maxo"], col = "#00ff0020")

```

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.

firstBaselineCheck,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 $\geq I$.
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 required for peaks with overlapping retention times; can be negative to allow overlap. During peak post-processing, peaks defined to be overlapping are reduced to the one peak with the largest signal.
fitgauss	logical(1) whether or not a Gaussian should be fitted to each peak. This affects mostly the retention time position of the 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. In detail, starting with a single m/z, a ROI is extended if a m/z can be found in the next scan (spectrum) for which the difference to the mean m/z of the ROI is smaller than the user defined ppm of the m/z. The mean m/z of the ROI is then updated considering also the newly included m/z value.

These ROIs are then, after some cleanup, 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.

[peaksWithCentWave](#) for functions to perform centWave peak detection in purely chromatographic data.

[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/K0", package = "faahKO"), recursive = TRUE,
           full.names = TRUE)
raw_data <- readMSData(flfs[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 m/z-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 (m/z 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.

<code>snthresh</code>	numeric(1) defining the signal to noise ratio cutoff.
<code>prefilter</code>	numeric(2): <code>c(k, I)</code> specifying the prefilter step for the first analysis step (ROI detection). Mass traces are only retained if they contain at least <code>k</code> peaks with intensity $\geq I$.
<code>mzCenterFun</code>	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.
<code>integrate</code>	Integration method. For <code>integrate = 1</code> peak limits are found through descent on the mexican hat filtered data, for <code>integrate = 2</code> 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.
<code>mzdiff</code>	numeric(1) representing the minimum difference in m/z dimension required for peaks with overlapping retention times; can be negative to allow overlap. During peak post-processing, peaks defined to be overlapping are reduced to the one peak with the largest signal.
<code>fitgauss</code>	logical(1) whether or not a Gaussian should be fitted to each peak. This affects mostly the retention time position of the peak.
<code>noise</code>	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).
<code>verboseColumns</code>	logical(1) whether additional peak meta data columns should be returned.
<code>roiList</code>	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: <code>scmin</code> (start scan index), <code>scmax</code> (end scan index), <code>mzmin</code> (minimum m/z), <code>mzmax</code> (maximum m/z), <code>length</code> (number of scans), <code>intensity</code> (summed intensity). Each ROI should be represented by a list of elements or a single row data.frame.
<code>firstBaselineCheck</code>	logical(1). If TRUE continuous data within regions of interest is checked to be above the first baseline.
<code>roiScales</code>	Optional numeric vector with length equal to <code>roiList</code> defining the scale for each region of interest in <code>roiList</code> that should be used for the <code>centWave</code> -wavelets.
<code>snthreshIsoROIs</code>	numeric(1) defining the signal to noise ratio cutoff to be used in the second <code>centWave</code> run to identify peaks for predicted isotope ROIs.
<code>maxCharge</code>	integer(1) defining the maximal isotope charge. Isotopes will be defined for charges <code>1:maxCharge</code> .
<code>maxIso</code>	integer(1) defining the number of isotope peaks that should be predicted for each peak identified in the first <code>centWave</code> run.
<code>mzIntervalExtension</code>	logical(1) whether the m/z range for the predicted isotope ROIs should be extended to increase detection of low intensity peaks.
<code>polarity</code>	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 specifies the minimum peak length in time scans. For withWave = TRUE the second argument represents the maximum peak length subject to being greater than the minimum 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 minimum 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 required for peaks with overlapping retention times; can be negative to allow overlap. During peak post-processing, peaks defined to be overlapping are reduced to the one peak with the largest signal.
fitgauss	logical(1) whether or not a Gaussian should be fitted to each peak. This affects mostly the retention time position of the 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 prediction 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 continuous 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 an 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 difficult 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(fl[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-derivative 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 $\min(mz) - \text{bin_size}/2$ and $\min(mz) + \text{bin_size}/2$).

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.

`peaksWithMatchedFilter` for functions to perform matchedFilter peak detection in purely chromatographic data.

`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 "XCMS²" 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 "XCMS²" 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="matchedFilter"). 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.methods`. 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 chosen 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

sntresh	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 (in the MassSpecWavelet) package is called to estimate the local intensity.
tuneIn	logical(1) whether 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 <code>msLevel = 1</code> .
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`, `n`
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	maximal 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 $(\text{maxo} - \text{baseline})/\text{sd}$, 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 Böttcher, 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	maximal 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 $(\text{maxo} - \text{baseline})/\text{sd}$, 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 <code>verbose.columns</code> 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
spos	Peak position found by wavelet analysis
smin	Left peak limit found by wavelet analysis (scan number)
smax	Right peak limit found by wavelet analysis (scan number)

Methods

```
object = "xcmsRaw" findPeaks.centWave(object, ppm=25, peakwidth=c(20,50), snthresh=10, pre
```

Author(s)

Ralf Tautenhahn

References

Ralf Tautenhahn, Christoph Bötter, 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	maximal 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 $(\text{maxo} - \text{baseline})/\text{sd}$, where <i>maxo</i> is the maximum peak intensity, <i>baseline</i> the estimated baseline value and <i>sd</i> the standard deviation of local chromatographic noise.
egauss	RMSE of Gaussian fit if <code>verbose.columns</code> 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 Böttcher, 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.

An xcmsRaw object.

criticalValue Numeric: Suggested values: (0.1-3.0). This setting helps determine the the Kalman Filter prediction 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 specifies 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 minimum 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 continuous 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 "scan-Back" 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 difficult 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(faahK0)
library(xcms)
#load all the wild type and Knock out samples
cdfpath <- system.file("cdf", package = "faahK0")
## 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, mzdifff = 0.8 - step * steps, index = FALSE, sleep = 0,
  scanrange = numeric())
```

Arguments

<code>object</code>	The <code>xcmsRaw</code> object on which peak detection should be performed.
<code>fwhm</code>	<code>numeric(1)</code> specifying the full width at half maximum of matched filtration gaussian model peak. Only used to calculate the actual sigma, see below.
<code>sigma</code>	<code>numeric(1)</code> specifying the standard deviation (width) of the matched filtration model peak.
<code>max</code>	<code>numeric(1)</code> representing the maximum number of peaks that are expected/will be identified per slice.
<code>snthresh</code>	<code>numeric(1)</code> defining the signal to noise cutoff to be used in the chromatographic peak detection step.
<code>step</code>	<code>numeric(1)</code> specifying the width of the bins/slices in m/z dimension.
<code>steps</code>	<code>numeric(1)</code> 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).
<code>mzdiff</code>	<code>numeric(1)</code> defining the minimum difference in m/z for peaks with overlapping retention times
<code>index</code>	<code>logical(1)</code> specifying whether indicies should be returned instead of values for m/z and retention times.
<code>sleep</code>	(DEPRECATED). The use of this parameter is highly discouraged, as it could cause problems in parallel processing mode.
<code>scanrange</code>	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 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 (\leq 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 MSⁿ Mass Spectrometry precursor peaks as annotated in XML raw file

Arguments

object xcmsRaw object

Details

Some mass spectrometers can acquire MS1 and MS2 (or MSⁿ scans) quasi simultaneously, e.g. in data dependent tandem MS or DDIT mode.

Since xcmsFragments attaches *all* MSⁿ 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 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 new user interface, [do_findPeaks_MS](#) 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 indices of peak groups for which to get EICs
sampleidx	either character vector with names or integer vector with indices 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 <code>xcmsSet</code> object
peakrange	matrix or data frame with 4 columns: <code>mzmin</code> , <code>mzmax</code> , <code>rtmin</code> , <code>rtmax</code> (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 (\leq 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	<i>Get m/z and intensity values for a single mass scan</i>
-----------------	--

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	<i>Get average m/z and intensity values for multiple mass scans</i>
-----------------	---

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	<i>Load the raw data for one or more files in the xcmsSet</i>
--------------------	---

Description

Reads the raw data applies eventual 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=1, ...)
```

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

<code>object</code>	xcmsSet-class object
<code>method</code>	Method to use for grouping. See details.
<code>...</code>	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	<i>Group peaks from different samples together</i>
---------------	--

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	<i>Group Peaks via High Resolution Alignment</i>
---------------	--

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	<i>Correspondence: Chromatographic peak grouping methods.</i>
-----------------	---

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	<i>Peak grouping based on time dimension peak densities</i>
-------------------------	---

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 m/z 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 <code>PeakDensityParam</code> 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 of the smoothing kernel) to be used. This argument is passed to the <code>density</code> 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 <code>groupChromPeaks</code> : an <code>XCMSnExp</code> object containing the results from a previous peak detection analysis (see <code>findChromPeaks</code>). For all other methods: a <code>PeakDensityParam</code> object.
value	The value for the slot.
param	A <code>PeakDensityParam</code> 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 the 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(fl[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 <code>PeakDensityParam</code> 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 <code>groupChromPeaks</code> : an <code>XCMSnExp</code> object containing the results from a previous chromatographic peak detection analysis (see <code>findChromPeaks</code>). For all other methods: a <code>MzClustParam</code> object.
value	The value for the slot.
param	A <code>MzClustParam</code> 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("fticrf", 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 <code>PeakDensityParam</code> 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 (euclidian) 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 <code>groupChromPeaks</code> : an <code>XCMSnExp</code> object containing the results from a previous chromatographic peak detection analysis (see <code>findChromPeaks</code>). For all other methods: a <code>NearestPeaksParam</code> object.
value	The value for the slot.
param	A <code>NearestPeaksParam</code> 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(flfs[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, XCMSnExp-method

Generate unique group (feature) names based on mass and retention time

Description

groupnames generates names for the identified features from the correspondence analysis based in their mass and retention time. This generates feature names that are equivalent to the group names of the *old* user interface (aka xcms1).

Usage

```
## S4 method for signature 'XCMSnExp'
groupnames(object, mzdec = 0, rtdec = 0,
           template = NULL)
```

Arguments

object	XCMSnExp object containing correspondence results.
mzdec	integer(1) with the number of decimal places to use for m/z (defaults to 0).
rtdec	integer(1) with the number of decimal places to use for the retention time (defaults to 0).
template	character with existing group names whose format should be emulated.

Value

character with unique names for each feature in object. The format is M(m/z)T(time in seconds).

See Also

[XCMSnExp](#).

groupnames-methods *Generate unique 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	<i>Add definition of chromatographic peaks to an extracted chromatogram plot</i>
---------------------	--

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",
  "polygon"), whichPeaks = c("any", "within", "apex_within"), ...)
```

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/peaks. 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 (if type = "rect") or the peak (for type = "polygon").
type	the plotting type. See plot in base graphics 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" and type = "polygon" will highlight the peak shape. For type = "polygon" the color of the border and area can be defined with parameters "border" and "col", respectively.

`whichPeaks` character(1) specifying how peaks are called to be located within the region defined by `mz` and `rt`. Can be one of "any", "within", and "apex_within" for all peaks that are even partially overlapping the region, peaks that are completely within the region, and peaks for which the apex is within the region. This parameter is passed to the `type` argument of the `chromPeaks` function. See related documentation for more information and examples.

... 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/K0/ko16.CDF', package = "faahKO"),
                   system.file('cdf/K0/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
## Show the peak definition with a rectangle
highlightChromPeaks(xod, rt = c(2700, 2900), mz = 335)

## Color the actual peak
highlightChromPeaks(xod, rt = c(2700, 2900), mz = 335,
                   col = c("#ff000020", "#00ff0020"), type = "polygon")
```

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

<code>x</code>	A numeric vector with eventual missing (NA) values.
<code>baseValue</code>	The base value to which empty elements should be set. This is only considered for <code>method = "linbase"</code> and corresponds to the <code>profBinLinBase</code> 's <code>baselevel</code> argument.
<code>method</code>	One of "none", "lin" or "linbase".
<code>distance</code>	For <code>method = "linbase"</code> : number of non-empty neighboring element of an empty element that should be considered for linear interpolation. See details section for more information.
<code>noInterpolAtEnds</code>	For <code>method = "lin"</code> : 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 (NAs 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, its value 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")

```

imputeRowMin

Replace missing values with a proportion of the row minimum

Description

imputeRowMin imputes missing values in `x` by replacing NAs in each row with a proportion of the minimal value for that row (i.e. `min_fraction * min(x[i,])`).

Usage

```
imputeRowMin(x, min_fraction = 1/2)
```

Arguments

<code>x</code>	matrix with abundances, rows being features/metabolites and columns samples.
<code>min_fraction</code>	numeric(1) with the fraction of the row minimum that should be used to replace NA values in that row.

Author(s)

Johannes Rainer

See Also

imputeLCMD package for more left censored imputation functions.
 Other imputation functions: [imputeRowMinRand](#)

Examples

```

library(faahKO)
data("faahko")

xset <- group(faahko)
mat <- groupval(xset, value = "into")

mat_imp <- imputeRowMin(mat)

head(mat)
head(mat_imp)

## Replace with 1/8 of the row minimum
head(imputeRowMin(mat, min_fraction = 1/8))

```

imputeRowMinRand	<i>Impute missing values with random numbers based on the row minimum</i>
------------------	---

Description

Replace missing values with random numbers from a normal distribution based on (a fraction of) the row min and a standard deviation estimated from the linear relationship between row standard deviation and mean of the full data set. Parameter `sd_fraction` allows to further reduce the estimated standard deviation.

Usage

```
imputeRowMinRand(x, min_fraction = 1/2, sd_fraction = 1, abs = TRUE)
```

Arguments

<code>x</code>	matrix with abundances, rows being features/metabolites and columns samples.
<code>min_fraction</code>	numeric(1) with the fraction of the row minimum that should be used to replace NA values in that row.
<code>sd_fraction</code>	numeric(1) factor to reduce the estimated standard deviation.
<code>abs</code>	logical(1) to force imputed values to be strictly positive.

Details

Imputed values are taken from a normal distribution with mean being a user defined fraction of the row minimum and the standard deviation estimated for that mean based on the linear relationship between row standard deviations and row means in the full matrix `x`.

To largely avoid imputed values being negative or larger than the *real* values, the standard deviation for the random number generation is estimated ignoring the intercept of the linear model estimating the relationship between standard deviation and mean. If `abs = TRUE` NA values are replaced with the absolute value of the random values.

Author(s)

Johannes Rainer

See Also

`imputeLCMD` package for more left censored imputation functions.

Other imputation functions: [imputeRowMin](#)

Examples

```
library(faahKO)
data("faahko")

xset <- group(faahko)
mat <- groupval(xset, value = "into")
```

```
## Estimate the relationship between row sd and mean. The standard deviation
## of the random distribution is estimated on this relationship.
mns <- rowMeans(mat, na.rm = TRUE)
sds <- apply(mat, MARGIN = 1, sd, na.rm = TRUE)
plot(mns, sds)
abline(lm(sds ~ mns))

mat_imp <- imputeRowMinRand(mat)

head(mat)
head(mat_imp)
```

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	whether 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	<i>Read binary data from a source</i>
-----------------	---------------------------------------

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 contains the following components:

<code>rt</code>	Numeric vector with acquisition time (in seconds) for each scan
<code>tic</code>	Numeric vector with Total Ion Count for each scan
<code>scanindex</code>	Integer vector with starting positions of each scan in the <code>mz</code> and <code>intensity</code> components. It is an exclusive offset, so <code>scanindex[i]</code> is the offset in <code>mz</code> and <code>intensity</code> <i>before</i> the beginning of scan <code>i</code> . This means that the <code>mz</code> (respectively <code>intensity</code>) values for scan <code>i</code> would be from <code>scanindex[i] + 1</code> to <code>scanindex[i + 1]</code>
<code>mz</code>	Concatenated vector of <code>m/z</code> values for all scans
<code>intensity</code>	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	<i>Apply a median filter to a matrix</i>
--------------	--

Description

For each element in a matrix, 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	<i>Copy MSn data in an xcmsRaw to the MS slots</i>
-------------	--

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")
```

overlappingFeatures *Identify overlapping features*

Description

overlappingFeatures identifies features that are overlapping or close in the m/z - rt space.

Usage

```
overlappingFeatures(x, expandMz = 0, expandRt = 0, ppm = 0)
```

Arguments

x	XCMSnExp with the features.
expandMz	numeric(1) with the value to expand each feature (on each side) in m/z dimension before identifying overlapping features. The resulting "mzmin" for the feature is thus $mzmin - expandMz$ and the "mzmax" $mzmax + expandMz$.
expandRt	numeric(1) with the value to expand each feature (on each side) in retention time dimension before identifying overlapping features. The resulting "rtmin" for the feature is thus $rtmin - expandRt$ and the "rtmax" $rtmax + expandRt$.
ppm	numeric(1) to grow the m/z width of the feature by a relative value: $mzmin - mzmin * ppm / 2e6$, $mzmax + mzmax * ppm / 2e6$. Each feature is thus expanded in m/z dimension by $ppm/2$ on each side before identifying overlapping features.

Value

list with indices of features (in [featureDefinitions\(\)](#)) that are overlapping.

Author(s)

Johannes Rainer

Examples

```
## Load 2 test files.
data <- readMSData(c(system.file("cdf/K0/ko15.CDF", package = "faahK0"),
                             system.file("cdf/K0/ko16.CDF", package = "faahK0")),
                  mode = "onDisk")

## Perform peak detection; parameters set to reduce processing speed
data <- findChromPeaks(data, CentWaveParam(noise = 10000, snthresh = 40))

## Correspondence analysis
data <- groupChromPeaks(data, param = PeakDensityParam(sampleGroups = c(1, 1)))

## Identify overlapping features
overlappingFeatures(data)

## Identify features that are separated on retention time by less than
## 2 minutes
overlappingFeatures(data, expandRt = 60)
```

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](#)

peaksWithCentWave *Identify peaks in chromatographic data using centWave*

Description

peaksWithCentWave identifies (chromatographic) peaks in purely chromatographic data, i.e. based on intensity and retention time values without m/z values.

Usage

```
peaksWithCentWave(int, rt, peakwidth = c(20, 50), snthresh = 10,
  prefilter = c(3, 100), integrate = 1, fitgauss = FALSE,
  noise = 0, verboseColumns = FALSE, firstBaselineCheck = TRUE, ...)
```

Arguments

int	numeric with intensity values.
rt	numeric with the retention time for the intensities. Length has to be equal to length(int).
peakwidth	numeric(2) with the lower and upper bound of the expected peak width.
snthresh	numeric(1) defining the signal to noise ratio cutoff. Peaks with a signal to noise ratio < snthresh are omitted.
prefilter	numeric(2) (c(k, I)): only regions of interest with at least k centroids with signal >= I are returned in the first step.
integrate	numeric(1), integration method. For integrate = 1 peak limits are found through descending on the mexican hat filtered data, for integrate = 2 the descend 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.
fitgauss	logical(1) whether or not a Gaussian should be fitted to each peak.
noise	numeric(1) defining the minimum required intensity for centroids to be considered in the first analysis step (definition of the <i>regions of interest</i>).
verboseColumns	logical(1): whether additional peak meta data columns should be returned.
firstBaselineCheck	logical(1). If TRUE continuous data within regions of interest is checked to be above the first baseline.
...	currently ignored.

Details

The method uses the same algorithm for the peak detection than [centWave](#), employs however a different approach to identify the initial regions in which the peak detection is performed (i.e. the *regions of interest* ROI). The method first identifies all local maxima in the chromatographic data and defines the corresponding positions +/- peakwidth[2] as the ROIs. Noise estimation bases also on these ROIs and can thus be different from [centWave](#) resulting in different signal to noise ratios.

Value

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

- "rt": retention time of the peak's midpoint (time of the maximum signal).
- "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 (original) intensity of the peak.
- "sn": signal to noise ratio of the peak defined as $(\text{maxo} - \text{baseline})/\text{sd}$ with sd being the standard deviation of the local chromatographic noise.

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 (always NA).
- "scale": scale on which the peak was localized.
- "scpos": peak position found by wavelet analysis (index in int).
- "scmin": left peak limit found by wavelet analysis (index in int).
- "scmax": right peak limit found by wavelet analysis (index in int).

Author(s)

Johannes Rainer

See Also

[centWave](#) for a detailed description of the peak detection method.

Other peak detection functions for chromatographic data: [peaksWithMatchedFilter](#)

Examples

```
## Reading a file
library(xcms)
od <- readMSData(system.file("cdf/K0/ko15.CDF", package = "faahK0"),
  mode = "onDisk")

## Extract chromatographic data for a small m/z range
mzr <- c(272.1, 272.2)
chr <- chromatogram(od, mz = mzr)[1, 1]

int <- intensity(chr)
rt <- rtime(chr)

## Plot the region
plot(chr, type = "h")
```

```
## Identify peaks in the chromatographic data
pks <- peaksWithCentWave(intensity(chr), rtime(chr))
pks

## Highlight the peaks
rect(xleft = pks[, "rtmin"], xright = pks[, "rtmax"],
     ybottom = rep(0, nrow(pks)), ytop = pks[, "maxo"], col = "#ff000040",
     border = "#00000040")
```

peaksWithMatchedFilter

Identify peaks in chromatographic data using matchedFilter

Description

The function performs peak detection using the [matchedFilter](#) algorithm on chromatographic data (i.e. with only intensities and retention time).

Usage

```
peaksWithMatchedFilter(int, rt, fwhm = 30, sigma = fwhm/2.3548,
                       max = 20, snthresh = 10, ...)
```

Arguments

int	numeric with intensity values.
rt	numeric with the retention time for the intensities. Length has to be equal to length(int).
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) with the maximal number of peaks that are expected/ will bbe detected in the data
snthresh	numeric(1) defining the signal to noise cut-off to be used in the peak detection step.
...	currently ignored.

Value

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

- "rt": retention time of the peak's midpoint (time of the maximum signal).
- "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 (original) intensity of the peak.
- "maxf": maximum intensity of the filtered peak.
- "sn": signal to noise ratio of the peak.

Author(s)

Johannes Rainer

See Also

[matchedFilter](#) for a detailed description of the peak detection method.

Other peak detection functions for chromatographic data: [peaksWithCentWave](#)

Examples

```
## Read one file from the faahKO package
od <- readMSData(system.file("cdf/K0/ko15.CDF", package = "faahKO"),
  mode = "onDisk")

## Extract chromatographic data for a small m/z range
chr <- chromatogram(od, mz = c(272.1, 272.3))[1, 1]

pks <- peaksWithMatchedFilter(intensity(chr), rtime(chr))
pks

## Plotting the data
plot(rtime(chr), intensity(chr), type = "h")
rect(xleft = pks[, "rtmin"], xright = pks[, "rtmax"], ybottom = c(0, 0),
  ytop = pks[, "maxo"], border = "red")
```

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 indices of peak groups for which to plot EICs

sampleidx either character vector with names or integer vector with indices 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 = xC`

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, ylim, ...)
```

Arguments

<code>object</code>	A XCMSnExp object with the alignment results.
<code>col</code>	colors to be used for the lines corresponding to the individual samples.
<code>lty</code>	line type to be used for the lines of the individual samples.
<code>type</code>	plot type to be used. See help on the <code>par</code> function for supported values.
<code>adjustedRtime</code>	logical(1) whether adjusted or raw retention times should be shown on the x-axis.
<code>xlab</code>	the label for the x-axis.
<code>ylab</code>	the label for the y-axis.
<code>peakGroupsCol</code>	color to be used for the peak groups (only used if alignment was performed using the adjustRtime-peakGroups method).
<code>peakGroupsPch</code>	point character (pch) to be used for the peak groups (only used if alignment was performed using the adjustRtime-peakGroups method).
<code>peakGroupsLty</code>	line type (lty) to be used to connect points for each peak groups (only used if alignment was performed using the adjustRtime-peakGroups method).
<code>ylim</code>	optional numeric(2) with the upper and lower limits on the y-axis.
<code>...</code>	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 indices 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, vline = NULL, ...)`

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, type = c("any", "within",
  "apex_within"), ...)
```

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 <i>peak density</i> correspondence algorithm can be extracted. If not provided and if object contains feature definitions with the correspondence/ peak grouping being performed by the <i>peak density</i> 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.
type	character(1) specifying how peaks are called to be located within the region defined by m/z and rt. Can be one of "any", "within", and "apex_within" for all peaks that are even partially overlapping the region, peaks that are completely within the region, and peaks for which the apex is within the region. This parameter is passed to the chromPeaks function. See related documentation for more information and examples.
...	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 m/z 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 m/z 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. 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 obiwarped
res <- adjustRtime(res, param = ObiwarpedParam())

## 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

plotChromPeaks 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	Specifies 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

DEPRECATED: Create a plot that combines a XIC and a mz/rt 2D plot for one sample

Description

UPDATE: please use `plot(x, type = "XIC")` from the MSnbase package instead. See examples below.

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

<code>x</code>	data.frame such as returned by the extractMsData() function. Only a single data.frame is supported.
<code>main</code>	character(1) specifying the title.
<code>cex</code>	numeric(1) defining the size of points. Passed directly to the plot function.
<code>mfrow</code>	numeric(2) defining the plot layout. This will be passed directly to <code>par(mfrow = mfrow)</code> . See <code>par</code> for more information. Setting <code>mfrow = NULL</code> avoids calling <code>par(mfrow = mfrow)</code> hence allowing to pre-define the plot layout.
<code>grid.color</code>	a color definition for the grid line (or NA to skip creating them).
<code>colramp</code>	a <i>color ramp palette</i> to be used to color the data points based on their intensity. See argument <code>col.regions</code> in lattice::level.colors documentation.

Author(s)

Johannes Rainer

Examples

```
## Read two files from the faahKO package
library(faahKO)
library(magrittr)
cdfs <- dir(system.file("cdf", package = "faahKO"), full.names = TRUE,
            recursive = TRUE)[1:2]
raw_data <- readMSData(cdfs, mode = "onDisk")

## Subset the object to a rt and mz range and plot the data.
raw_data %>%
  filterRt(rt = c(2700, 2900)) %>%
  filterMz(mz = c(334.9, 335.1)) %>%
  plot(type = "XIC")
```

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	<i>Plot m/z and RT deviations for QC purposes without external reference data</i>
--------	---

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 m/z 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 "mzdev-time": Shows whether m/z deviations are RT dependent, could indicate instrument drift "mzdevsample": median m/z deviation for each sample, indicates outliers "rtdevsample": median RT deviation for each sample, indicates outliers

Details

plotQC() is a wrapper to create a set of diagnostic plots. For the m/z deviations, the median of all m/z within one group are assumed.

Value

List with four matrices, each of dimension features * samples: "mz": median m/z deviation for each sample "mzdev": median m/z 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	<i>Plot mass spectra from the profile matrix</i>
------------------	--

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 indices 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	<i>Plot profile matrix 3D surface using OpenGL</i>
------------------	--

Description

This method uses the `rgl` package to create interactive three dimensional 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

<code>object</code>	the xcmsRaw object
<code>ident</code>	logical, use mouse to identify and label chromatographic peaks
<code>msident</code>	logical, use mouse to identify and label spectral peaks

Value

If `ident == TRUE`, an integer vector with the indices 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 defining 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 $n \times m$ 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 / step). See distance parameter of imputeLinInterpol for more details.
mzrange.	Optional numeric(2) manually specifying the mz value range to be used for binning. 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 setting 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 following 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 start and 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(), scanrange = numeric(), masslab = character(), scanlab = character(), massidx = integer(), scanidx = integer(), timelab = character(), timeidx = integer(), ...)

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(faahK0)
cdfpath <- system.file("cdf", package = "faahK0")
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

<code>object</code>	xcmsRaw object
<code>mzrange</code>	m/z range for EIC
<code>rtrange</code>	retention time range for EIC
<code>scanrange</code>	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	<i>Get a raw data matrix</i>
----------------	------------------------------

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 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 retention 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	matrix 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](#)

rla	<i>Calculate relative log abundances rla calculates the relative log abundances (RLA, see reference) on a numeric vector.</i>
-----	---

Description

Calculate relative log abundances

rla calculates the relative log abundances (RLA, see reference) on a numeric vector.

rowRla calculates row-wise RLAs.

Usage

```
rla(x, group, log.transform = TRUE)
```

```
rowRla(x, group, log.transform = TRUE)
```

Arguments

x numeric (for rla) or matrix (for rowRla) with the abundances (in natural scale) on which the RLA should be calculated.

group factor, numeric or character with the same length than x that groups values in x. If omitted all values are considered to be from the same group.

log.transform logical(1) whether x should be log2 transformed. Set to log.transform = FALSE if x is already in log scale.

Details

The RLA is defines as the (log) abundance of an analyte relative to the median across all abundances of the same group.

Value

numeric of the same length than x (for rla) or matrix with the same dimensions than x (for rowRla).

Author(s)

Johannes Rainer

References

De Livera AM, Dias DA, De Souza D, Rupasinghe T, Pyke J, Tull D, Roessner U, McConville M, Speed TP. Normalizing and integrating metabolomics data. *Anal Chem* 2012 Dec 18;84(24):10768-76.

Examples

```
x <- c(3, 4, 5, 1, 2, 3, 7, 8, 9)
grp <- c(1, 1, 1, 2, 2, 2, 3, 3, 3)
r1a(x, grp)
```

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

<code>object</code>	a <code>xcmsSet</code> or <code>xcmsRaw</code> .
<code>method</code>	Method to use for distance calculation. See details.
<code>...</code>	<code>mzabs</code> , <code>mzppm</code> 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="meanMZmatch")`. This is also the default.

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

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

Value

<code>mzabs</code>	maximum absolute deviation for two matching peaks
<code>mzppm</code>	relative deviations in ppm for two matching peaks
<code>symmetric</code>	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	<i>a Distance function based on matching peaks</i>
-----------------	--

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, nPmin=0)
```

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 peaktables

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 = 0.001)
```

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 considered 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	<i>Identify peaks in a sparse continuum mode spectrum</i>
-----------	---

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 <i>mz</i> and <i>intensity</i>
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:

<i>mz</i>	m/z at maximum peak intensity
<i>intensity</i>	maximum intensity of the peak
<i>fwhm</i>	full width at half max of the peak

Author(s)

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

See Also

[getSpec](#), [specNoise](#)

split.xcmsRaw	<i>Divide an xcmsRaw object</i>
---------------	---------------------------------

Description

Divides the scans from a xcmsRaw object into a list of multiple objects. MSⁿ 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	<i>Divide an xcmsSet object</i>
---------------	---------------------------------

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 evaluates the Gaussian model and its gradient. It has an `initial` attribute that will evaluate the initial estimates of the parameters `mu`, `sigma`, and `h`.

Usage

```
SSgauss(x, mu, sigma, h)
```

Arguments

<code>x</code>	a numeric vector of values at which to evaluate the model
<code>mu</code>	mean of the distribution function
<code>sigma</code>	standard deviation of the distribution function
<code>h</code>	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 $h \cdot \sqrt{2 \cdot \pi}$.

Value

A numeric vector of the same length as `x`. It is the value of the expression $h \cdot \exp(-(x-\mu)^2 / (2 \cdot \sigma^2))$, 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 <code>xcmsRaw-class</code> 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(faahK0) ## These files do not have this problem to correct for but just for an example
cdfpath <- system.file("cdf", package = "faahK0")
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 equal
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 <i>xcmsSet</i> 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 are affected by this option are:

- [do_findChromPeaks_matchedFilter](#): use the original code that iteratively creates a subset of the binned (profile) matrix. This is helpful for computers with limited memory or matched-Filter settings with a very small bin size.
- [getPeaks](#)

Value

logical(1) indicating whether old code is being used.

Note

For parallel processing using the SOCKS method (e.g. by [SnowParam\(\)](#) on Windows computers) this option might not be passed to the individual R processes performing the calculations. In such cases it is suggested to specify the option manually and system-wide by adding the line `options(XCMSuseOriginalCode = TRUE)` in a file called *.Rprofile* in the folder in which new R processes are started (usually the user's home directory; to ensure that the option is correctly read add a new line to the file too). See also [Startup](#) from the base R documentation on how to specify system-wide options for R.

Usage of old code is strongly discouraged. 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 schema, see <http://www.psidev.info/mzquantml>

Value

None.

See Also

[write.mzQuantML](#)

<code>write.cdf-methods</code>	<i>Save an <code>xcmsRaw</code> object to file</i>
--------------------------------	--

Description

Write the raw data to a (simple) CDF file.

Arguments

<code>object</code>	the <code>xcmsRaw</code> object
<code>filename</code>	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.psdev.info/mzquantml>

Value

None.

Methods

```
object = "xcmsSet" write.mzQuantML(object, filename)
```

See Also

[xcmsSet-class](#), [xcmsSet](#), [verify.mzQuantML](#),

writeMSData, XCMSnExp, character-method

Export MS data to mzML/mzXML files

Description

writeMSData exports mass spectrometry data in mzML or mzXML format. If adjusted retention times are present, these are used as retention time of the exported spectra.

Usage

```
## S4 method for signature 'XCMSnExp,character'  
writeMSData(object, file,  
  outformat = c("mzml", "mzxml"), copy = FALSE,  
  software_processing = NULL, ...)
```

Arguments

object	XCMSnExp object with the mass spectrometry data.
file	character with the file name(s). The length of this parameter has to match the number of files/samples of object.
outformat	character(1) defining the format of the output files (either "mzml" or "mzxml").
copy	logical(1) if metadata (data processing, software used, original file names etc) should be copied from the original files.
software_processing	optionally provide specific data processing steps. See documentation of the software_processing parameter of mzR::writeMSData() .
...	Additional parameters to pass down to the writeMSData() function in the MSnbase package, such as outformat to specify the output format ("mzml" or "mzxml") or copy to specify whether general information from the original MS data files (such as data processing, software etc) should be copied to the new files.

Author(s)

Johannes Rainer

See Also

[writeMSData\(\)](#) function in the MSnbase package.

`writeMzTab`*Save a grouped xcmsSet object in mzTab-1.1 format file*

Description

Write the grouped xcmsSet to an mzTab file.

Arguments

<code>object</code>	the xcmsSet object
<code>filename</code>	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.
- `extractMsData`: replaced by `as(x, "data.frame")`.
- `plotMsData`: replaced by `plot(x, type = "XIC")`.

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 matrices 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**EXPERIMENTAL 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 MSⁿ 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 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

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 MSⁿ 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 MSⁿ 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 columns 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 a container for the results of a G/LC-MS preprocessing that comprises chromatographic peak detection, alignment and correspondence. These results can be accessed with the `chromPeaks`, `adjustedRtime` and `featureDefinitions` functions; see below (after the Usage, Arguments, Value and Slots sections) for more details). 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. XCMSnExp objects, by directly extending the `OnDiskMSnExp` object from the MSnbase package, inherit all of its functionality and allows thus an easy access to the full raw data at any stage of an analysis. To support interaction with packages requiring the *old* objects, XCMSnExp objects can be coerced into `xcmsSet` objects using the `as` method (see examples below). All preprocessing results will be passed along to the resulting `xcmsSet` object.

General functions for XCMSnExp objects are:

`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).

`hasFilledChromPeaks`: whether filled-in peaks are present or not.

`profMat`: creates a *profile matrix*, which is a $n \times m$ 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 m/z - rt features (peak groups). Similar to the `chromPeaks` it is possible to extract features for specified m/z and/or rt ranges. The function supports also the parameter `type` that allows to specify which features to be returned if any of `rt` or `mz` is specified. For details see help of `chromPeaks`. See also `featureSummary` for a function to calculate simple feature summaries.

`chromPeaks`, `chromPeaks<-`: extract or set the matrix containing the information on identified chromatographic peaks. Rownames of the matrix represent unique IDs of the respective peaks within the experiment. 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`, `ppm` and `type` allow to extract only chromatographic peaks overlapping the defined retention time and/or `m/z` ranges. Argument `type` allows to define how *overlapping* is determined: for `type == "any"` (the default), all peaks that are even partially overlapping the region are returned, for `type == "within"` the full peak has to be within the region and for `type == "apex_within"` the peak's apex position (highest signal of the peak) has to be within the region. 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.

`rttime`: 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` ob-

jects 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.

`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.

XCMSnExp objects can be combined with the `c` function. This combines identified chromatographic peaks and the objects' pheno data but discards alignment results or feature definitions.

Usage

```
processHistoryTypes()

hasFilledChromPeaks(object)

## S4 method for signature 'OnDiskMSEnExp'
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 = c("any", "within", "apex_within"))

## 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 = c("any",
  "within", "apex_within"))

## 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(), ...)

## S3 method for class 'XCMSnExp'
c(...)

```

Arguments

object For `adjustedRtime`, `featureDefinitions`, `chromPeaks`, `hasAdjustedRtime`, `hasFeatures` and `hasChromPeaks` either a `MsFeatureData` or a `XCMSnExp` ob-

	ject, 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 $2 * \text{basespace}$ 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 $\text{distance} = \text{floor}(\text{basespace} / \text{step})$. See distance parameter of imputeLinInterpol for more details.
mzrange.	Optional numeric(2) manually specifying the mz value range to be used for binning. 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 $\text{mz}[1] - \text{ppm} / 1\text{e}6$ and $\text{mz}[2] + \text{ppm} / 1\text{e}6$ 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 partially overlapping the range defined by mz and/or rt are returned, type = "within" returns only peaks completely within the region and type = "apex_within" peaks for which the peak's apex is within the region.
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 (each row being a chromatographic peak, row-names representing unique IDs of the peaks) 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 intensity 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 chromatographic 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.

Chromatographic peak data

Chromatographic peak data is added to an `XCMSnExp` object by the [findChromPeaks](#) function. Functions to access chromatographic peak data are:

- `hasChromPeaks` whether chromatographic peak data is available, see below for help of the function.
- `chromPeaks` access chromatographic peaks (see below for help).
- `dropChromPeaks` remove chromatographic peaks (see below for help).
- `dropFilledChromPeaks` remove filled-in peaks (see below for help).
- [fillChromPeaks](#) fill-in missing peaks (see respective help page).
- [plotChromPeaks](#) plot identified peaks for a file (see respective help page).
- [plotChromPeakImage](#) plot distribution of peaks along the retention time axis (see respective help page).
- [highlightChromPeaks](#) add chromatographic peaks to an existing plot of a [Chromatogram](#) (see respective help page).

Adjusted retention times

Adjusted retention times are stored in an `XCMSnExp` object besides the original, raw, retention times, allowing to switch between raw and adjusted times. It is also possible to replace the raw retention times with the adjusted ones with the [applyAdjustedRtime](#). The adjusted retention times are added to an `XCMSnExp` by the [adjustRtime](#) function. All functions related to the access of adjusted retention times are:

- `hasAdjustedRtime` whether adjusted retention times are available (see below for help).
- `dropAdjustedRtime` remove adjusted retention times (see below for help).
- [applyAdjustedRtime](#) replace the raw retention times with the adjusted ones (see respective help page).
- [plotAdjustedRtime](#) plot differences between adjusted and raw retention times (see respective help page).

Correspondence results, features

The correspondence analysis ([groupChromPeaks](#)) adds the feature definitions to an `XCMSnExp` object. All functions related to these are listed below:

- `hasFeatures` whether correspondence results are available (see below for help).

- `featureDefinitions` access the definitions of the features (see below for help).
- `dropFeatureDefinitions` remove correspondence results (see below for help).
- `featureValues` access values for features (see respective help page).
- `featureSummary` perform a simple summary of the defined features (see respective help page).
- `link{overlappingFeatures}` identify features that are overlapping or close in the m/z - rt space (see respective help page).

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.

`as` (`as(x, "data.frame")`) in the `MSnbase` package for the method to extract MS data as `data.frames`.

`featureSummary` to calculate basic feature summaries.

`featureChromatograms` to extract chromatograms for each feature.

`chromPeakSpectra` to extract MS2 spectra with the m/z of the precursor ion within the m/z range of a peak and a retention time within its retention time range.

`featureSpectra` to extract MS2 spectra associated with identified features.

`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 identified 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_commdata = 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_commdata	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/you/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@acadiu.ca>, modified by Ralf Tautenhahn <rtautenh@ipb-halle.de>.

References

<http://ace.acadiu.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	<i>A matrix of peaks</i>
-----------------	--------------------------

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 or 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 m/z 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.psivdev.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 representation 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`: character 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 sub-setted). 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	<i>DEPRECATED</i> , 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 extension 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	<i>Virtual class for raw data sources</i>
------------------	---

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	<i>Create an xcmsSource object in a flexible way</i>
--------------------	--

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](#)

```
[,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

<code>x</code>	The <code>xcmsRaw</code> object that should be sub-setted.
<code>i</code>	Integer or logical vector specifying the scans/spectra to which <code>x</code> should be sub-setted.
<code>j</code>	Not supported.
<code>drop</code>	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/K0/ko15.CDF', package = "faahK0")
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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