Package 'xcms'

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Title LC-MS and GC-MS Data Analysis

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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'do_adjustRtime-functions.R' 'functions-binning.R'
'do_findChromPeaks-functions.R' 'functions-Params.R'
'do_groupChromPeaks-functions.R' 'fastMatch.R'
'functions-Chromatogram.R' 'functions-utils.R' 'functions-IO.R'
'functions-OnDiskMSnExp.R' 'functions-ProcessHistory.R'
'functions-XCMSnExp.R' 'functions-imputation.R'
'functions-xcmsEIC.R' 'functions-xcmsFragments.R'
'functions-xcmsRaw.R' 'functions-xcmsSet.R'
'functions-xcmsSwath.R' 'init.R' 'loadXcmsData.R'
'matchpeaks.R' 'method-filterFeatures.R'
'methods-Chromatogram.R' 'methods-IO.R'
'methods-MChromatograms.R' 'methods-MsFeatureData.R'
'methods-OnDiskMSnExp.R' 'methods-Params.R'
'methods-ProcessHistory.R' 'methods-XCMSnExp.R'
'methods-XChromatogram.R' 'methods-XChromatograms.R'
'methods-group-features.R' 'methods-xcmsEIC.R'
'methods-xcmsFileSource.R' 'methods-xcmsFragments.R'
'methods-xcmsPeaks.R' 'methods-xcmsRaw.R' 'methods-xcmsSet.R'
'models.R' 'mzClust.R' 'plotQC.R' 'ramp.R' 'specDist.R'
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Contents

absent-methods 7
adjustRtime 7
adjustRtime,XcmsExperiment,LamaParama-method 15

applyAdjustedRtime . . . 18
AutoLockMass-methods . . . 20
bin,XCMSnExp-method . . . 21
binYonX . . . 23
BlankFlag . . . 26
breaks_on_binSize . . . 28
breaks_on_nBins . . . 29
c-methods . . . 30
CalibrantMassParam-class . . . 31
calibrate-methods . . . 33
chromatogram,XCMSnExp-method . . . 34
chromPeakChromatograms . . . 37
chromPeakSpectra . . . 38
collect-methods . . . 42
colMax . . . 43
correlate,Chromatogram,Chromatogram-method . . . 44
descendZero . . . 46
diffreport-methods . . . 47
dirname . . . 49
doubleMatrix . . . 49
do_adjustRtime_peakGroups . . . 50
do_findChromPeaks_centWave . . . 52
do_findChromPeaks_centWaveWithPredIsoROIs . . . 56
do_findChromPeaks_massifquant . . . 61
do_findChromPeaks_matchedFilter . . . 64
do_findPeaks_MSW . . . 67
do_groupChromPeaks_density . . . 69
do_groupChromPeaks_nearest . . . 72
do_groupPeaks_mzClust . . . 73
DratioFilter . . . 75
estimatePrecursorIntensity . . . 76
etg . . . 77
exportMetaboAnalyst . . . 78
extractMsData,OnDiskMSnExp-method . . . 79
feature-grouping . . . 81
featureChromatograms . . . 82
featureSpectra . . . 85
featureSummary . . . 87
fillChromPeaks . . . 89
fillPeaks-methods . . . 94
fillPeaks.chrom-methods . . . 95
fillPeaks.MSW-methods . . . 96
filterColumnsIntensityAbove,MChromatograms-method . . . 97
filterFeatureDefinitions . . . 99
filterFeatures . . . 115
filtfft . . . 117
findChromPeaks . . . 117
findChromPeaks,Chromatogram,CentWaveParam-method . . . 119

findChromPeaks,Chromatogram,MatchedFilterParam-method . . . 121
findChromPeaks-centWave . . . 122
findChromPeaks-centWaveWithPredIsoROIs . . . 128
findChromPeaks-massifquant . . . 133
findChromPeaks-matchedFilter . . . 140
findChromPeaksIsolationWindow . . . 145
findEqualGreater . . . 147
findMZ . . . 148
findneutral . . . 149
findPeaks-methods . . . 151
findPeaks-MSW . . . 152
findPeaks.addPredictedIsotopeFeatures-methods . . . 156
findPeaks.centWave-methods . . . 159
findPeaks.centWaveWithPredictedIsotopeROIs-methods . . . 161
findPeaks.massifquant-methods . . . 164
findPeaks.matchedFilter,xcmsRaw-method . . . 166
findPeaks.MS1-methods . . . 168
findPeaks.MSW,xcmsRaw-method . . . 170
GenericParam-class . . . 171
getEIC-methods . . . 172
getPeaks-methods . . . 173
getScan-methods . . . 174
getSpec-methods . . . 174
getXcmsRaw-methods . . . 175
group-methods . . . 176
group.density . . . 177
group.mzClust . . . 178
group.nearest . . . 179
groupChromPeaks . . . 180
groupFeatures-abundance-correlation . . . 186
groupFeatures-eic-similarity . . . 187
groupFeatures-similar-rtime . . . 191
groupnames,XCMSnExp-method . . . 192
groupnames-methods . . . 193
groupOverlaps . . . 193
groupval-methods . . . 194
highlightChromPeaks . . . 195
image-methods . . . 197
imputeLinInterpol . . . 197
imputeRowMin . . . 199
imputeRowMinRand . . . 200
isolationWindowTargetMz,OnDiskMSnExp-method . . . 202
levelplot-methods . . . 203
loadRaw-methods . . . 203
loadXcmsData . . . 204
manualChromPeaks . . . 205
medianFilter . . . 208
msn2xcmsRaw . . . 209

na.flatfill . . . 210
overlappingFeatures . . . 210
panel.cor . . . 211
peakPlots-methods . . . 212
peaksWithCentWave . . . 213
peaksWithMatchedFilter . . . 215
peakTable-methods . . . 217
PercentMissingFilter . . . 218
phenoDataFromPaths . . . 219
PlainTextParam . . . 220
plot.xcmsEIC . . . 222
plotAdjustedRtime . . . 223
plotChrom-methods . . . 225
plotChromatogramsOverlay . . . 225
plotChromPeakDensity,XCMSnExp-method . . . 228
plotChromPeaks . . . 231
plotEIC-methods . . . 233
plotFeatureGroups . . . 234
plotMsData . . . 235
plotPeaks-methods . . . 236
plotQC . . . 236
plotRaw-methods . . . 238
plotrt-methods . . . 238
plotScan-methods . . . 239
plotSpec-methods . . . 240
plotSurf-methods . . . 240
plotTIC-methods . . . 241
ProcessHistory-class . . . 242
profGenerate . . . 243
profMat,MsExperiment-method . . . 245
profMedFilt-methods . . . 248
profMethod-methods . . . 248
profRange-methods . . . 249
profStep-methods . . . 250
pval . . . 251
quantify,XCMSnExp-method . . . 251
rawEIC-methods . . . 253
rawMat-methods . . . 254
RDataParam . . . 255
reconstructChromPeakSpectra . . . 256
rectUnique . . . 258
refineChromPeaks . . . 259
removeIntensity,Chromatogram-method . . . 263
retcor-methods . . . 265
retcor.obiwarp . . . 266
retcor.peakgroups-methods . . . 267
retexp . . . 268
rla . . . 268

RsdFilter . . . 269
sampnames-methods . . . 271
showError,xcmsSet-method . . . 271
specDist-methods . . . 272
specDist.cosine . . . 273
specDist.meanMZmatch . . . 274
specDist.peakCount-methods . . . 275
specNoise . . . 275
specPeaks . . . 276
split.xcmsRaw . . . 277
split.xcmsSet . . . 278
SSgauss . . . 278
stitch-methods . . . 279
storeResults . . . 281
updateObject,xcmsSet-method . . . 282
useOriginalCode . . . 282
verify.mzQuantM . . . 283
write.cdf-methods . . . 284
write.mzdata-methods . . . 285
write.mzQuantML-methods . . . 285
writeMSData,XCMSnExp,character-method . . . 286
writeMzTab . . . 287
XChromatograms . . . 288
xcms-deprecated . . . 300
xcmsEIC-class . . . 301
xcmsFileSource-class . . . 302
xcmsFragments . . . 303
xcmsFragments-class . . . 304
XCMSnExp-class . . . 305
xcmsPeaks-class . . . 316
xcmsRaw . . . 317
xcmsRaw-class . . . 319
xcmsSet . . . 321
xcmsSet-class . . . 323
xcmsSource-class . . . 326
xcmsSource-methods . . . 327
[,XCMSnExp,ANY,ANY,ANY-method . . . 327
[,xcmsRaw,logicalOrNumeric,missing,missing-method . . . 332

Index **334**

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

Description

Determine which peaks are absent / present in a sample class

Arguments

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

Details

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

Value

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

Methods

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

See Also

group diffreport

adjustRtime *Alignment: Retention time correction methods.*

Description

The adjustRtime method(s) perform retention time correction (alignment) between chromatograms of different samples/dataset. Alignment is performed by default on MS level 1 data. Retention times of spectra from other MS levels, if present, are subsequently adjusted based on the adjusted retention times of the MS1 spectra. Note that calling adjustRtime on a *xcms* result object will remove any eventually present previous alignment results as well as any correspondence analysis results. To run a second round of alignment, raw retention times need to be replaced with adjusted ones using the applyAdjustedRtime() function.

The alignment method can be specified (and configured) using a dedicated param argument.

Supported param objects are:

- `ObiwarpParam`: performs retention time adjustment based on the full m/z - rt data using the *obiwarp* method (Prince (2006)). It is based on the original code but supports in addition 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.
- `PeakGroupsParam`: performs retention time correction based on the alignment of features defined in all/most samples (corresponding to *house keeping compounds* or marker compounds) (Smith 2006). First the retention time deviation of these features is described by fitting either a polynomial (`smooth = "loess"`) or a linear (`smooth = "linear"`) function to the data points. These are then subsequently used to adjust the retention time of each spectrum in each sample (even from spectra of MS levels different than MS 1). Since the function is based on features (i.e. chromatographic peaks grouped across samples) a initial correspondence analysis has to be performed **before** using the `groupChromPeaks()` function. Alternatively, it is also possible to manually define a `numeric` matrix with retention times of markers in each samples that should be used for alignment. Such a `matrix` can be passed to the alignment function using the `peakGroupsMatrix` parameter of the `PeakGroupsParam` parameter object. By default the `adjustRtimePeakGroups` function is used to define this `matrix`. This function identifies peak groups (features) for alignment in `object` based on the parameters defined in `param`. See also `do_adjustRtime_peakGroups()` for the core API function.
- `LamaParama`: This function performs retention time correction by aligning chromatographic data to an external reference dataset (concept and initial implementation by Carl Brunius). The process involves identifying and aligning peaks within the experimental chromatographic data, represented as an `XcmsExperiment` object, to a predefined set of landmark features called "lamas". These landmark features are characterized by their mass-to-charge ratio (m/z) and retention time. see `LamaParama()` for more information on the method.

Usage

```
adjustRtime(object, param, ...)

## S4 method for signature 'MsExperiment,ObiwarpParam'
adjustRtime(object, param, chunkSize = 2L, BPPARAM = bpparam())

## S4 method for signature 'MsExperiment,PeakGroupsParam'
adjustRtime(object, param, msLevel = 1L, ...)

PeakGroupsParam(
  minFraction = 0.9,
  extraPeaks = 1,
  smooth = "loess",
  span = 0.2,
  family = "gaussian",
  peakGroupsMatrix = matrix(nrow = 0, ncol = 0),
  subset = integer(),
  subsetAdjust = c("average", "previous")
)

ObiwarpParam(
```

```
  binSize = 1,
  centerSample = integer(),
  response = 1L,
  distFun = "cor_opt",
  gapInit = numeric(),
  gapExtend = numeric(),
  factorDiag = 2,
  factorGap = 1,
  localAlignment = FALSE,
  initPenalty = 0,
  subset = integer(),
  subsetAdjust = c("average", "previous"),
  rtimeDifferenceThreshold = 5
)

adjustRtimePeakGroups(object, param = PeakGroupsParam(), msLevel = 1L)

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

## 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 'PeakGroupsParam'
subset(x)

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

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

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

## 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 'ObiwarpParam'
subset(x)

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

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

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

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

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

```
adjustRtime(object, param, msLevel = 1L)
```

Arguments

object	For adjustRtime: an OnDiskMSnExp(), XCMSnExp(), MsExperiment() or XcmsExperiment() object.
param	The parameter object defining the alignment method (and its setting).
...	ignored.
chunkSize	For adjustRtime if object is either an MsExperiment or XcmsExperiment: integer(1) defining the number of files (samples) that should be loaded into memory and processed at the same time. Alignment is then performed in parallel (per sample) on this subset of loaded data. This setting thus allows to balance between memory demand and speed (due to parallel processing). Because parallel processing can only performed on the subset of data currently loaded into memory in each iteration, the value for chunkSize should match the defined parallel setting setup. Using a parallel processing setup using 4 CPUs (separate processes) but using chunkSize = 1will not perform any parallel processing, as only the data fr to the total number of samples in an experiment will load the full MS data into memory and will thus in most settings cause an out-of-memory error.
BPPARAM	parallel processing setup. Defaults to BPPARAM = bpparam(). See bpparam() for details.
msLevel	For adjustRtime: integer(1) defining the MS level on which the alignment should be performed.
minFraction	For PeakGroupsParam: numeric(1) between 0 and 1 defining the minimum required proportion 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. Note that if subset is provided, the specified fraction is relative to the defined subset of samples and not to the total number of samples within the experiment (i.e., a peak has to be present in the specified proportion of subset samples).
extraPeaks	For PeakGroupsParam: numeric(1) defining the maximal number of additional peaks for all samples to be assigned to a peak group (feature) for retention time correction. For a data set with 6 samples, extraPeaks = 1 uses all peak groups with a total peak count <= 6 + 1. The total peak count is the total number of peaks being assigned to a peak group and considers also multiple peaks within a sample that are assigned to the group.
smooth	For PeakGroupsParam: character(1) defining the function to be used to interpolate corrected retention times for all peak groups. Can be either "loess" or "linear".
span	For PeakGroupsParam: numeric(1) defining the degree of smoothing (if smooth = "loess"). This parameter is passed to the internal call to loess().
family	For PeakGroupsParam: character(1) defining the method for loess smoothing. Allowed values are "gaussian" and "symmetric". See loess() for more information.

peakGroupsMatrix
: For PeakGroupsParam: optional matrix of (raw) retention times for the (marker) peak groups on which the alignment should be performed. Each column represents a sample, each row a feature/peak group. The adjustRtimePeakGroups method is used by default to determine this matrix on the provided object.

subset
: For ObiwarpParam and PeakGroupsParam: integer with the indices of samples within the experiment on which the alignment models should be estimated. Samples not part of the subset are adjusted based on the closest subset sample. See *Subset-based alignment* section for details.

subsetAdjust
: For ObiwarpParam and PeakGroupsParam: character(1) specifying the method with which non-subset samples should be adjusted. Supported options are "previous" and "average" (default). See *Subset-based alignment* section for details.

binSize
: numeric(1) defining the bin size (in mz dimension) to be used for the *profile matrix* generation. See step parameter in profile-matrix documentation for more details.

centerSample
: integer(1) defining the index of the center sample in the experiment. It defaults to floor(median(1:length(fileNames(object)))). Note that if subset is used, the index passed with centerSample is within these subset samples.

response
: For ObiwarpParam: numeric(1) defining the *responsiveness* of warping with response = 0 giving linear warping on start and end points and response = 100 warping using all bijective anchors.

distFun
: For ObiwarpParam: character(1) defining the distance function to be used. Allowed values are "cor" (Pearson's correlation), "cor_opt" (calculate only 10% diagonal band of distance matrix; better runtime), "cov" (covariance), "prd" (product) and "euc" (Euclidian distance). The default value is distFun = "cor_opt".

gapInit
: For ObiwarpParam: numeric(1) defining the penalty for gap opening. The default value for depends on the value of distFun: distFun = "cor" and distFun = "cor_opt" it is 0.3, for distFun = "cov" and distFun = "prd" 0.0 and for distFun = "euc" 0.9.

gapExtend
: For ObiwarpParam: numeric(1) defining the penalty for gap enlargement. The default value for gapExtend depends on the value of distFun: for distFun = "cor" and distFun = "cor_opt" it is 2.4, distFun = "cov" 11.7, for distFun = "euc" 1.8 and for distFun = "prd" 7.8.

factorDiag
: For ObiwarpParam: numeric(1) defining the local weight applied to diagonal moves in the alignment.

factorGap
: For ObiwarpParam: numeric(1) defining the local weight for gap moves in the alignment.

localAlignment
: For ObiwarpParam: logical(1) whether a local alignment should be performed instead of the default global alignment.

initPenalty
: For ObiwarpParam: numeric(1) defining the penalty for initiating an alignment (for local alignment only).

rtimeDifferenceThreshold
: For ObiwarpParam: numeric(1) defining the threshold to identify a *gap* in the sequence of retention times of (MS1) spectra of a sample/file. A gap is defined if

the difference in retention times between consecutive spectra is > rtimeDifferenceThreshold of the median observed difference or retenion times of that data sample/file. Spectra with an retention time after such a *gap* will not be adjusted. The default for this parameter is rtimeDifferenceThreshold = 5. For Waters data with lockmass scans or LC-MS/MS data this might however be a too low threshold and it should be increased. See also issue #739.

value — The value for the slot.

x — An ObiwarpParam, PeakGroupsParam or LamaParama object.

Value

adjustRtime on an OnDiskMSnExp or XCMSnExp object will return an XCMSnExp object with the alignment results.

adjustRtime on an MsExperiment or XcmsExperiment will return an XcmsExperiment with the adjusted retention times stored in an new *spectra variable* rtime_adjusted in the object's spectra.

ObiwarpParam, PeakGroupsParam and LamaParama return the respective parameter object.

adjustRtimeGroups returns a matrix with the retention times of *marker* features in each sample (each row one feature, each row one sample).

Subset-based alignment

All alignment methods allow to perform the retention time correction on a user-selected subset of samples (e.g. QC samples) after which all samples not part of that subset will be adjusted based on the adjusted retention times of the *closest* subset sample (close in terms of index within object and hence possibly injection index). It is thus suggested to load MS data files in the order in which their samples were injected in the measurement run(s).

How the non-subset samples are adjusted depends also on the parameter subsetAdjust: with subsetAdjust = "previous", each non-subset sample is adjusted based on the closest *previous* subset sample which results in most cases with adjusted retention times of the non-subset sample being identical to the subset sample on which the adjustment bases. The second, default, option is subsetAdjust = "average" in which case each non subset sample is adjusted based on the average retention time adjustment from the previous and following subset sample. For the average, a weighted mean is used with weights being the inverse of the distance of the non-subset sample to the subset samples used for alignment.

See also section *Alignment of experiments including blanks* in the *xcms* vignette for more details.

Author(s)

Colin Smith, Johannes Rainer, Philippine Louail, Carl Brunius

References

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

Smith, C.A., Want, E.J., O'Maille, G., Abagyan, R. and Siuzdak, G. (2006). "XCMS: Processing Mass Spectrometry Data for Metabolite Profiling Using Nonlinear Peak Alignment, Matching, and Identification" *Anal. Chem.* 78:779-787.

See Also

plotAdjustedRtime() for visualization of alignment results.

`adjustRtime,XcmsExperiment,LamaParama-method`
Landmark-based alignment: aligning a dataset against an external reference

---

Description

Alignment is achieved using the ['adjustRtime()'] method with a 'param' of class 'LamaParama'. This method corrects retention time by aligning chromatographic data with an external reference dataset.

Chromatographic peaks in the experimental data are first matched to predefined (external) landmark features based on their mass-to-charge ratio and retention time and subsequently the data is aligned by minimizing the differences in retention times between the matched chromatographic peaks and lamas. This adjustment is performed file by file.

Adjustable parameters such as 'ppm', 'tolerance', and 'toleranceRt' define acceptable deviations during the matching process. It's crucial to note that only lamas and chromatographic peaks exhibiting a one-to-one mapping are considered when estimating retention time shifts. If a file has no peaks matching with lamas, no adjustment will be performed, and the the retention times will be returned as-is. Users can evaluate this matching, for example, by checking the number of matches and ranges of the matching peaks, by first running '[matchLamasChromPeaks()]'.

Different warping methods are available; users can choose to fit a *loess* ('method = "loess"', the default) or a *gam* ('method = "gam"') between the reference data points and observed matching ChromPeaks. Additional parameters such as 'span', 'weight', 'outlierTolerance', 'zeroWeight', and 'bs' are specific to these models. These parameters offer flexibility in fine-tuning how the matching chromatographic peaks are fitted to the lamas, thereby generating a model to align the overall retention time for a single file.

Other functions related to this method:

- 'LamaParama()': return the respective parameter object for alignment using 'adjustRtime()' function. It is also the input for the functions listed below.

- 'matchLamasChromPeaks()': quickly matches each file's ChromPeaks to Lamas, allowing the user to evaluate the matches for each file.

- 'summarizeLamaMatch()': generates a summary of the 'LamaParama' method. See below for the details of the return object.

- 'matchedRtimes()': Access the list of 'data.frame' saved in the 'LamaParama' object, generated by the 'matchLamasChromPeaks()' function.

- 'plot()':plot the chromatographic peaks versus the reference lamas as well as the fitting line for the chosen model type. The user can decide what file to inspect by specifying the assay number with the parameter 'assay'

Usage

```
## S4 method for signature 'XcmsExperiment,LamaParama'
adjustRtime(object, param, BPPARAM = bpparam(), ...)

matchLamasChromPeaks(object, param, BPPARAM = bpparam())

summarizeLamaMatch(param)

matchedRtimes(param)

LamaParama(
  lamas = matrix(ncol = 2, nrow = 0, dimnames = list(NULL, c("mz", "rt"))),
  method = c("loess", "gam"),
  span = 0.5,
  outlierTolerance = 3,
  zeroWeight = 10,
  ppm = 20,
  tolerance = 0,
  toleranceRt = 5,
  bs = "tp"
)

## S4 method for signature 'LamaParama,ANY'
plot(
  x,
  index = 1L,
  colPoints = "#00000060",
  colFit = "#00000080",
  xlab = "Matched Chromatographic peaks",
  ylab = "Lamas",
  ...
)
```

Arguments

object	An object of class ‘XcmsExperiment‘ with defined ChromPeaks.
param	An object of class ‘LamaParama‘ that will later be used for adjustment using the ‘[adjustRtime()]‘ function.
BPPARAM	For ‘matchLamasChromPeaks()‘: parallel processing setup. Defaults to ‘BPPARAM = bpparam()‘. See [bpparam()] for more information.
...	For ‘plot()‘: extra parameters to be passed to the function.
lamas	For ‘LamaParama‘: ‘matrix‘ or ‘data.frame‘ with the m/z and retention times values of features (as first and second column) from the external dataset on which the alignment will be based on.
method	For ‘LamaParama‘:‘character(1)‘ with the type of warping. Either ‘method = "gam"‘ or ‘method = "loess"‘ (default).

span	For ‘LamaParama‘: ‘numeric(1)‘ defining the degree of smoothing (‘method = "loess"‘). This parameter is passed to the internal call to [loess()].
outlierTolerance	For ‘LamaParama‘: ‘numeric(1)‘ defining the settings for outlier removal during the fitting. By default (with ‘outlierTolerance = 3‘), all data points with absolute residuals larger than 3 times the mean absolute residual of all data points from the first, initial fit, are removed from the final model fit.
zeroWeight	For ‘LamaParama‘: ‘numeric(1)‘: defines the weight of the first data point (i.e. retention times of the first lama-chromatographic peak pair). Values larger than 1 reduce warping problems in the early RT range.
ppm	For ‘LamaParama‘: ‘numeric(1)‘ defining the m/z-relative maximal allowed difference in m/z between ‘lamas‘ and chromatographic peaks. Used for the mapping of identified chromatographic peaks and lamas.
tolerance	For ‘LamaParama‘: ‘numeric(1)‘ defining the absolute acceptable difference in m/z between lamas and chromatographic peaks. Used for the mapping of identified chromatographic peaks and ‘lamas‘.
toleranceRt	For ‘LamaParama‘: ‘numeric(1)‘ defining the absolute acceptable difference in retention time between lamas and chromatographic peaks. Used for the mapping of identified chromatographic peaks and ‘lamas‘.
bs	For ‘LamaParama()‘: ‘character(1)‘ defining the GAM smoothing method. (defaults to thin plate, ‘bs = "tp"‘)
x	For ‘plot()‘: object of class ‘LamaParama‘ to be plotted.
index	For ‘plot()‘: ‘numeric(1)‘ index of the file that should be plotted.
colPoints	For ‘plot()‘: color for the plotting of the datapoint.
colFit	For ‘plot()‘: color of the fitting line.
xlab, ylab	For ‘plot()‘: x- and y-axis labels.

Value

For ‘matchLamasChromPeaks()‘: A ‘LamaParama‘ object with new slot ‘rtMap‘ composed of a list of matrices representing the 1:1 matches between Lamas (ref) and ChromPeaks (obs). To access this, ‘matchedRtimes()‘ can be used.

For ‘matchedRtimes()‘: A list of ‘data.frame‘ representing matches between chromPeaks and ‘lamas‘ for each files.

For ‘summarizeLamaMatch()‘:A ‘data.frame‘ with:

- "Total_peaks": total number of chromatographic peaks in the file.

- "Matched_peak": The number of matched peaks to Lamas.

- "Total_Lamas": Total number of Lamas.

- "Model_summary": ‘summary.loess‘ or ‘summary.gam‘ object for each file.

Note

If there are no matches when using ‘matchLamasChromPeaks()‘, the file retention will not be adjusted when calling [adjustRtime()] with the same ‘LamaParama‘ and ‘XcmsExperiment‘ object.

To see examples on how to utilize this methods and its functionality, see the vignette.

Author(s)

Carl Brunius, Philippine Louail

Examples

```
## load test and reference datasets
ref <- loadXcmsData("xmse")
tst <- loadXcmsData("faahko_sub2")

## create lamas input from the reference dataset
library(MsExperiment)
f <- sampleData(ref)$sample_type
f[f == "QC"] <- NA
ref <- filterFeatures(ref, PercentMissingFilter(threshold = 0, f = f))
ref_mz_rt <- featureDefinitions(ref)[, c("mzmed","rtmed")]

## Set up the LamaParama object
param <- LamaParama(lamas = ref_mz_rt, method = "loess", span = 0.5,
                    outlierTolerance = 3, zeroWeight = 10, ppm = 20,
                    tolerance = 0, toleranceRt = 20, bs = "tp")

## input into `adjustRtime()`
tst_adjusted <- adjustRtime(tst, param = param)

## run diagnostic functions to pre-evaluate alignment
param <- matchLamasChromPeaks(tst, param = param)
mtch <- matchedRtimes(param)

## Access summary of matches and model information
summary <- summarizeLamaMatch(param)

##coverage for each file
summary$Matched_peaks / summary$Total_peaks * 100

## Access the information on the model of for the first file
summary$model_summary[[1]]
```

---

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 or XcmsExperiment object.

Details

Adjusted retention times are stored *in parallel* to the adjusted retention times in XCMSnExp or XcmsExperiment objects. The applyAdjustedRtime replaces the raw (original) retention times with the adjusted retention times.

Value

An XCMSnExp or XcmsExperiment object with the raw (original) 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 a test data set with detected peaks
library(MSnbase)
data(faahko_sub)
## Update the path to the files for the local system
dirname(faahko_sub) <- system.file("cdf/KO", package = "faahKO")

## Disable parallel processing for this example
register(SerialParam())

xod <- adjustRtime(faahko_sub, 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(faahko_sub), fromFile(faahko_sub))[[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(x, 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

x	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.
object	XCMSnExp or OnDiskMSnExp object.
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.

Value

For all methods: a XCMSnExp object.

Author(s)

Johannes Rainer

See Also

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

---

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

Description

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

Usage

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

Arguments

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

Details

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

binFromX and binToX allow to overwrite this by manually defining the a range on which the breaks should be calculated. See examples below for more details.

Calculation of breaks: for nBins the breaks correspond to seq(min(x[fromIdx])), max(x[fromIdx], length.out = (nBins + 1)). For binSize the breaks correspond to seq(min(x[fromIdx]), max(x[toIdx]), by = binSize) with the exception that the last break value is forced to be equal to max(x[toIdx]). This ensures that all values from the specified range are covered by the breaks defining the bins. The last bin could however in some instances be slightly larger than binSize. See breaks_on_binSize and breaks_on_nBins for more details.

Value

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

Note

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

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

Author(s)

Johannes Rainer

See Also

imputeLinInterpol

Examples

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

```
## (in this example 1 and 12) fall within a bin, i.e. 12 is considered for
## the last bin.

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

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

#######
## Bin in overlapping sub-sets of X
##
## In this example we define overlapping sub-sets of X and perform the binning
## within these.
X <- 1:30
## Define the start and end indices of the sub-sets.
fIdx <- c(2, 8, 21)
tIdx <- c(10, 25, 30)
binYonX(X, nBins = 5L, fromIdx = fIdx, toIdx = tIdx)
## The same, but pre-defining also the desired range of the bins.
binYonX(X, nBins = 5L, fromIdx = fIdx, toIdx = tIdx, binFromX = 4, binToX = 28)
## The same bins are thus used for each sub-set.
```

BlankFlag *Flag features based on the intensity in blank samples*

Description

The ‘BlankFlag‘ class and method enable users to flag features of an ‘XcmsExperiment‘ or ‘SummarizedExperiment‘ object based on the relationship between the intensity of a feature in blanks compared to the intensity in the samples.

This class and method are part of the possible dispatch of the generic function ‘filterFeatures‘. Features *below* (‘<‘) the user-input threshold will be flagged by calling the ‘filterFeatures‘ function. This means that an extra column will be created in ‘featureDefinitions‘ or ‘rowData‘ called ‘possible_contaminants‘ with a logical value for each feature.

Usage

```
BlankFlag(
  threshold = 2,
  blankIndex = integer(),
  qcIndex = integer(),
  na.rm = TRUE
)

## S4 method for signature 'XcmsResult,BlankFlag'
filterFeatures(object, filter, ...)

## S4 method for signature 'SummarizedExperiment,BlankFlag'
filterFeatures(object, filter, assay = 1)
```

Arguments

`threshold`	‘numeric‘ indicates the minimum difference required between the mean abundance of a feature in samples compared to the mean abundance of the same feature in blanks for it to not be considered a possible contaminant. For example, the default threshold of 2 signifies that the mean abundance of the features in samples has to be at least twice the mean abundance in blanks for it to not be flagged as a possible contaminant.
`blankIndex`	‘integer‘ (or ‘logical‘) vector corresponding to the indices of blank samples.
`qcIndex`	‘integer‘ (or ‘logical‘) vector corresponding to the indices of quality control (QC) samples.
`na.rm`	‘logical‘ indicates whether missing values (‘NA‘) should be removed prior to the calculations.
`object`	`XcmsExperiment` or `SummarizedExperiment`. For an `XcmsExperiment` object, the `featureValues(object)` will be evaluated, and for `Summarizedesxperiment` the `assay(object, assay)`. The object will be filtered.
`filter`	The parameter object selecting and configuring the type of filtering. It can be one of the following classes: `RsdFilter`, `DratioFilter`, `PercentMissingFilter` or `BlankFlag`.
`...`	Optional parameters. For `object` being an `XcmsExperiment`: parameters for the `featureValues()` call.

assay — For filtering of SummarizedExperiment objects only. Indicates which assay the filtering will be based on. Note that the features for the entire object will be removed, but the computations are performed on a single assay. Default is 1, which means the first assay of the object will be evaluated.

Value

For 'BlankFlag': a 'BlankFlag' class. 'filterFeatures' returns the input object with an added column in the features metadata called 'possible_contaminants' with a logical value for each feature. This is added to 'featureDefinitions' for 'XcmsExperiment' objects and 'rowData' for 'SummarizedExperiment' objects.

Author(s)

Philippine Louail

See Also

Other Filter features in xcms: DratioFilter, PercentMissingFilter, RsdFilter

---

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

Description

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

Usage

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

Arguments

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

Details

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

Value

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

Author(s)

Johannes Rainer

See Also

binYonX for a binning function.

Other functions to define bins: breaks_on_nBins()

Examples

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

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

---

breaks_on_nBins *Generate breaks for binning*

Description

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

Usage

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

Arguments

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

Details

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

Value

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

Author(s)

Johannes Rainer

See Also

`binYonX` for a binning function.

Other functions to define bins: `breaks_on_binSize()`

Examples

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

---

c-methods *Combine xcmsSet objects*

Description

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

Arguments

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

Value

A `xcmsSet` object.

Methods

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

Author(s)

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

See Also

xcmsSet-class

CalibrantMassParam-class

Calibrant mass based calibration of chromatgraphic peaks

Description

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

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

Usage

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

isCalibrated(object)

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

Arguments

`mz`	a `numeric` or `list` of `numeric` vectors with reference mz values. If a `numeric` vector is provided, this is used for each sample in the `XCMSnExp` object. If a `list` is provided, it's length has to be equal to the number of samples in the experiment.
`mzabs`	`numeric(1)` the absolute error/deviation for matching peaks to calibrants (in Da).
`mzppm`	`numeric(1)` the relative error for matching peaks to calibrants in ppm (parts per million).

neighbors	integer(1) with the maximal number of peaks within the permitted distance to the calibrants that are considered. Among these the mz value of the peak with the largest intensity is used in the calibration function estimation.
method	character(1) defining the method that should be used to estimate the calibration function. Can be "shift", "linear" (default) or "edgeshift".
object	An XCMSnExp object.
param	The CalibrantMassParam object with the calibration settings.

Details

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

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

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

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

Value

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

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

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

Note

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

Author(s)

Joachim Bargsten, Johannes Rainer

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

Description

Calibrate peaks of a xcmsSet via a set of known masses

Arguments

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

Value

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

Methods

object = "xcmsSet" `calibrate(object, calibrants,method="linear", mzabs=0.0001, mzppm=5, neighbours=3, plotres=FALSE)`

See Also

`xcmsSet-class`,

chromatogram,XCMSnExp-method
Extracting chromatograms

Description

chromatogram: extract chromatographic data (such as an extracted ion chromatogram, a base peak chromatogram or total ion chromatogram) from an OnDiskMSnExp or XCMSnExp objects. See also the help page of the chromatogram function 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),
  filled = FALSE,
  include = c("apex_within", "any", "none"),
  ...
)
```

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.
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.
aggregationFun	character(1) specifying the function to be used to aggregate intensity values across the mz value range for the same retention time. Allowed values are "sum" (the default), "max", "mean" and "min".
missing	numeric(1) allowing to specify the intensity value to be used if for a given retention time no signal was measured within the mz range of the corresponding scan. Defaults to NA_real_ (see also Details and Notes sections below). Use missing = 0 to resemble the behaviour of the getEIC from the *old* user interface.

msLevel	integer(1) 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 MChromatograms object. Adjusted retention times are used by default if available.
filled	logical(1) whether filled-in peaks should also be returned. Defaults to filled = FALSE, i.e. returns only detected chromatographic peaks in the result object.
include	character(1) defining which chromatographic peaks should be returned. Supported are include = "apex_within" (the default) which returns chromatographic peaks that have their apex within the mz rt range, include = "any" to return all chromatographic peaks which m/z and rt ranges overlap the mz and rt or include = "none" to not include any chromatographic peaks.
...	optional parameters - currently ignored.

Details

Arguments rt and mz allow to specify the MS data slice (i.e. the m/z range and retention time window) from which the chromatogram should be extracted. These parameters can be either a numeric of length 2 with the lower and upper limit, or a matrix with two columns with the lower and upper limits to extract multiple EICs at once. 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).

If for a given retention time no intensity is measured in that spectrum a NA intensity value is returned by default. This can be changed with the parameter missing, setting missing = 0 would result in a 0 intensity being returned in these cases.

Value

chromatogram returns a XChromatograms 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). All chromatographic peaks with their apex position within the m/z and retention time range are also retained as well as all feature definitions for these peaks.

Note

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 changed by setting adjustedRtime = FALSE.

Author(s)

Johannes Rainer

See Also

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

[XChromatograms] for the object allowing to arrange
multiple [XChromatogram] objects.

[plot] to plot a [XChromatogram] or [MChromatograms] objects.

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

Examples

```
## Load a test data set with identified chromatographic peaks
library(MSnbase)
data(faahko_sub)
## Update the path to the files for the local system
dirname(faahko_sub) <- system.file("cdf/KO", package = "faahKO")

## Disable parallel processing for this example
register(SerialParam())

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

chrs

## Identified chromatographic peaks
chromPeaks(chrs)

## Plot the chromatogram
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(faahko_sub, mz = mzr, rt = rtr)

chromPeaks(chrs)

plot(chrs)

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

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

chromPeakChromatograms *Extract an ion chromatogram for each chromatographic peak*

Description

Extract an ion chromatogram (EIC) for each chromatographic peak in an XcmsExperiment() object. The result is returned as an XChromatograms() of length equal to the number of chromatographic peaks (and one column).

Usage

```
chromPeakChromatograms(object, ...)

## S4 method for signature 'XcmsExperiment'
chromPeakChromatograms(
  object,
  expandRt = 0,
  expandMz = 0,
  aggregationFun = "max",
  peaks = character(),
  return.type = c("XChromatograms", "MChromatograms"),
  ...,
  progressbar = TRUE
)
```

Arguments

object	An XcmsExperiment() with identified chromatographic peaks.
...	currently ignored.
expandRt	numeric(1) to eventually expand the retention time range from which the signal should be integrated. The chromatogram will contain signal from chromPeaks[, "rtmin"] - expandRt to chromPeaks[, "rtmax"] + expandRt. The default is expandRt = 0.
expandMz	numeric(1) to eventually expand the m/z range from which the signal should be integrated. The chromatogram will contain signal from chromPeaks[, "mzmin"] - expandMz to chromPeaks[, "mzmax"] + expandMz. The default is expandMz = 0.
aggregationFun	character(1) defining the function how signals within the m/z range in each spectrum (i.e. for each discrete retention time) should be aggregated. The default (aggregationFun = "max") reports the largest signal for each spectrum.
peaks	optional character providing the IDs of the chromatographic peaks (i.e. the row names of the peaks in chromPeaks(object)) for which chromatograms should be returned.

return.type	character(1) specifying the type of the returned object. Can be either return.type = "XChromatograms" (the default) or return.type = "MChromatograms" to return either a chromatographic object with or without the identified chromatographic peaks, respectively.
progressbar	logical(1) whether the progress of the extraction process should be displayed.

Author(s)

Johannes Rainer

See Also

featureChromatograms() to extract an EIC for each feature.

Examples

```
## Load a test data set with detected peaks
library(MSnbase)
library(xcms)
library(MsExperiment)
faahko_sub <- loadXcmsData("faahko_sub2")

## Get EICs for every detected chromatographic peak
chrs <- chromPeakChromatograms(faahko_sub)
chrs

## Order of EICs matches the order in chromPeaks
chromPeaks(faahko_sub) |> head()

## variable "sample_index" provides the index of the sample the EIC was
## extracted from
fData(chrs)$sample_index

## Get the EIC for selected peaks only.
pks <- rownames(chromPeaks(faahko_sub))[c(6, 12)]
pks

## Expand the data on retention time dimension by 15 seconds (on each side)
res <- chromPeakChromatograms(faahko_sub, peaks = pks, expandRt = 5)
plot(res[1, ])
```

---

chromPeakSpectra *Extract spectra associated with chromatographic peaks*

Description

Extract (MS1 or MS2) spectra from an XcmsExperiment or XCMSnExp object for identified chromatographic peaks. To return spectra for selected chromatographic peaks, their *peak ID* (i.e., row name in the chromPeaks matrix) can be provided with parameter peaks. For msLevel = 1L (only

supported for return.type = "Spectra" or return.type = "List") MS1 spectra within the retention time boundaries (in the file in which the peak was detected) are returned. For msLevel = 2L MS2 spectra are returned for a chromatographic peak if their precursor m/z is within the retention time and m/z range of the chromatographic peak. Parameter method allows to define whether all or a single spectrum should be returned:

- method = "all": (default): return all spectra for each chromatographic peak.
- method = "closest_rt": return the spectrum with the retention time closest to the peak's retention time (at apex).
- method = "closest_mz": return the spectrum with the precursor m/z closest to the peaks's m/z (at apex); only supported for msLevel > 1.
- method = "largest_tic": return the spectrum with the largest total signal (sum of peaks intensities).
- method = "largest_bpi": return the spectrum with the largest peak intensity (maximal peak intensity).
- method = "signal": only for object being a XCMSnExp: return the spectrum with the sum of intensities most similar to the peak's apex signal ("maxo"); only supported for msLevel = 2L.

Parameter return.type allows to specify the *type* of the result object. With return.type = "Spectra" (the default) a Spectra object with all matching spectra is returned. The spectra variable "peak_id" of the returned Spectra contains the ID of the chromatographic peak (i.e., the rowname of the peak in the chromPeaks matrix) for each spectrum. With return.type = "Spectra" a List of Spectra is returned. The length of the list is equal to the number of rows of chromPeaks. Each element of the list contains thus a Spectra with all spectra for one chromatographic peak (or a Spectra of length 0 if no spectrum was found for the respective chromatographic peak).

See also the *LC-MS/MS data analysis* vignette for more details and examples.

Usage

```
chromPeakSpectra(object, ...)

## S4 method for signature 'XcmsExperiment'
chromPeakSpectra(
  object,
  method = c("all", "closest_rt", "closest_mz", "largest_tic", "largest_bpi"),
  msLevel = 2L,
  expandRt = 0,
  expandMz = 0,
  ppm = 0,
  skipFilled = FALSE,
  peaks = character(),
  return.type = c("Spectra", "List"),
  BPPARAM = bpparam()
)

## S4 method for signature 'XCMSnExp'
chromPeakSpectra(
  object,
```

```
  msLevel = 2L,
  expandRt = 0,
  expandMz = 0,
  ppm = 0,
 method = c("all", "closest_rt", "closest_mz", "signal", "largest_tic", "largest_bpi"),
  skipFilled = FALSE,
  return.type = c("Spectra", "MSpectra", "List", "list"),
  peaks = character()
)
```

Arguments

object	XcmsExperiment or XCMSnExp object with identified chromatographic peaks for which spectra should be returned.
...	ignored.
method	character(1) specifying which spectra to include in the result. Defaults to method = "all". See function description for details.
msLevel	integer(1) defining the MS level of the spectra that should be returned.
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.
skipFilled	logical(1) whether spectra for filled-in peaks should be reported or not.
peaks	character, logical or integer allowing to specify a subset of chromatographic peaks in chromPeaks for which spectra should be returned (providing either their ID, a logical vector same length than nrow(chromPeaks(x)) or their index in chromPeaks(x)). This parameter overrides skipFilled.
return.type	character(1) defining the type of result object that should be returned.
BPPARAM	parallel processing setup. Defaults to bpparam().

Value

parameter return.type allow to specify the type of the returned object:

- return.type = "Spectra" (default): a Spectra object (defined in the Spectra package). The result contains all spectra for all peaks. Metadata column "peak_id" provides the ID of the respective peak (i.e. its rowname in chromPeaks().
- return.type = "List": List of length equal to the number of chromatographic peaks is returned, each element being a Spectra with the spectra for one chromatographic peak.

For backward compatibility options "MSpectra" and "list" are also supported but are not suggested.

- return.type = "MSpectra" (deprecated): a MSpectra object with elements being Spectrum objects. The result objects contains all spectra for all peaks. Metadata column "peak_id" provides the ID of the respective peak (i.e. its rowname in chromPeaks()).

- 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

Examples

```
## Read a file with DDA LC-MS/MS data
library(MsExperiment)
fl <- system.file("TripleTOF-SWATH/PestMix1_DDA.mzML", package = "msdata")

dda <- readMsExperiment(fl)

## Perform MS1 peak detection
dda <- findChromPeaks(dda, CentWaveParam(peakwidth = c(5, 15),
    prefilter = c(5, 1000)))

## Return all MS2 spectro for each chromatographic peaks as a Spectra object
ms2_sps <- chromPeakSpectra(dda)
ms2_sps

## spectra variable *peak_id* contain the row names of the peaks in the
## chromPeak matrix and allow thus to map chromatographic peaks to the
## returned MS2 spectra
ms2_sps$peak_id
chromPeaks(dda)

## Alternatively, return the result as a List of Spectra objects. This list
## is parallel to chromPeaks hence the mapping between chromatographic peaks
## and MS2 spectra is easier.
ms2_sps <- chromPeakSpectra(dda, return.type = "List")
names(ms2_sps)
rownames(chromPeaks(dda))
ms2_sps[[1L]]

## Parameter `msLevel` allows to define from which MS level spectra should
## be returned. By default `msLevel = 2L` but with `msLevel = 1L` all
## MS1 spectra with a retention time within the retention time range of
## a chromatographic peak can be returned. Alternatively, selected
## spectra can be returned by specifying the selection criteria/method
## with the `method` parameter. Below we extract for each chromatographic
## peak the MS1 spectra with a retention time closest to the
## chromatographic peak's apex position. Alternatively it would also be
## possible to select the spectrum with the highest total signal or
## highest (maximal) intensity.
ms1_sps <- chromPeakSpectra(dda, msLevel = 1L, method = "closest_rt")
ms1_sps

## Parameter peaks would allow to extract spectra for specific peaks only.
## Peaks can be defined with parameter `peaks` which can be either an
## `integer` with the index of the peak in the `chromPeaks` matrix or a
```

```
## `character` with its rowname in `chromPeaks`.
chromPeakSpectra(dda, msLevel = 1L, method = "closest_rt", peaks = c(3, 5))
```

---

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

Description

Collecting Peaks into xcmsFragmentss 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, ...)`

colMax *Find row and column maximum values*

Description

Find row and column maximum values for numeric arrays.

Usage

```
colMax(x, na.rm = FALSE, dims = 1)
rowMax(x, na.rm = FALSE, dims = 1)
which.colMax(x, na.rm = FALSE, dims = 1)
which.rowMax(x, na.rm = FALSE, dims = 1)
```

Arguments

x	an array of two or more dimensions, containing numeric values
na.rm	logical. Should missing values (including 'NaN') be omitted from the calculations? (not currently implemented)
dims	Which dimensions are regarded as "rows" or "columns" to maximize. For rowMax, the maximum is over dimensions dims+1, ...; for colMax it is over dimensions 1:dims.

Details

These functions are designed to act like the colSums series of functions except that they only currently handle real arrays and will not remove NA values.

Value

A numeric array of suitable size, or a vector if the result is one-dimensional. The dimnames (or names for a vector result) are taken from the original array.

For the which.* functions, an integer array of suitable size, or a vector if the result is one-dimensional. The indecies returned are for accessing x one-dimensionally (i.e. x[index]). For which.colMax(), the actual row indecies my be determined using (which.colMax(x)-1) %% nrow(x) + 1. For which.rowMax(), the actual column indecies may be determined using ceiling(rowMax(x)/nrow(x)).

Author(s)

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

See Also

colSums

`correlate,Chromatogram,Chromatogram-method`
Correlate chromatograms

Description

For `xcms` **>= 3.15.3 please use** `compareChromatograms()` **instead of** `correlate`

Correlate intensities of two chromatograms with each other. If the two `Chromatogram` objects have different retention times they are first *aligned* to match data points in the first to data points in the second chromatogram. See help on `alignRt` in `MSnbase::Chromatogram()` for more details.

If `correlate` is called on a single `MChromatograms()` object a pairwise correlation of each chromatogram with each other is performed and a `matrix` with the correlation coefficients is returned.

Note that the correlation of two chromatograms depends also on their order, e.g. `correlate(chr1, chr2)` might not be identical to `correlate(chr2, chr1)`. The lower and upper triangular part of the correlation matrix might thus be different.

Usage

```
## S4 method for signature 'Chromatogram,Chromatogram'
correlate(
  x,
  y,
  use = "pairwise.complete.obs",
  method = c("pearson", "kendall", "spearman"),
  align = c("closest", "approx"),
  ...
)

## S4 method for signature 'MChromatograms,missing'
correlate(
  x,
  y = NULL,
  use = "pairwise.complete.obs",
  method = c("pearson", "kendall", "spearman"),
  align = c("closest", "approx"),
  ...
)

## S4 method for signature 'MChromatograms,MChromatograms'
correlate(
  x,
  y = NULL,
  use = "pairwise.complete.obs",
  method = c("pearson", "kendall", "spearman"),
  align = c("closest", "approx"),
  ...
```

)

Arguments

x	Chromatogram() or MChromatograms() object.
y	Chromatogram() or MChromatograms() object.
use	character(1) passed to the cor function. See cor() for details.
method	character(1) passed to the cor function. See cor() for details.
align	character(1) defining the alignment method to be used. See help on alignRt in MSnbase::Chromatogram() for details. The value of this parameter is passed to the method parameter of alignRt.
...	optional parameters passed along to the alignRt method such as tolerance that, if set to 0 requires the retention times to be identical.

Value

numeric(1) or matrix (if called on MChromatograms objects) with the correlation coefficient. If a matrix is returned, the rows represent the chromatograms in x and the columns the chromatograms in y.

Author(s)

Michael Witting, Johannes Rainer

Examples

```
library(MSnbase)
chr1 <- Chromatogram(rtime = 1:10 + rnorm(n = 10, sd = 0.3),
    intensity = c(5, 29, 50, NA, 100, 12, 3, 4, 1, 3))
chr2 <- Chromatogram(rtime = 1:10 + rnorm(n = 10, sd = 0.3),
    intensity = c(80, 50, 20, 10, 9, 4, 3, 4, 1, 3))
chr3 <- Chromatogram(rtime = 3:9 + rnorm(7, sd = 0.3),
    intensity = c(53, 80, 130, 15, 5, 3, 2))

chrs <- MChromatograms(list(chr1, chr2, chr3))

## Using `compareChromatograms` instead of `correlate`.
compareChromatograms(chr1, chr2)
compareChromatograms(chr2, chr1)

compareChromatograms(chrs, chrs)
```

descendZero *Find start and end points of a peak*

Description

Decends down the sides of a data peak and finds either the points greater than or equal to the zero intercept, the intercept with a given value, or the bottom of the first valley on each side.

Usage

```
descendZero(y, istart = which.max(y))
descendValue(y, value, istart = which.max(y))
descendMin(y, istart = which.max(y))
```

Arguments

y	numeric vector with values
istart	starting point for descent
value	numeric value to descend to

Value

An integer vector of length 2 with the starting and ending indicies of the peak start and end points.

Author(s)

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

See Also

descendValue

Examples

```
normdist <- dnorm(seq(-4, 4, .1)) - .1
xcms:::descendZero(normdist)
normdist[xcms:::descendZero(normdist)]
xcms:::descendValue(normdist, .15)
normdist[xcms:::descendValue(normdist, .15)]
xcms:::descendMin(normdist)
```

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 from the multtest package.

Details

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

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

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

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

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

Value

A data frame with the following columns:

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

Methods

object = "xcmsSet" `diffreport(object, class1 = levels(sampclass(object))[1], class2 = levels(sampclass(object))[2], filebase = character(), eicmax = 0, eicwidth = 200, sortpval = TRUE, classeic = c(class1,class2), value=c("into","maxo","intb"), metlin = FALSE, h=480,w=640, mzdec=2, missing = numeric(), ...)`

See Also

xcmsSet-class, palette

---

dirname *Change the file path of an* OnDiskMSnExp *object*

Description

dirname allows to get and set the path to the directory containing the source files of the OnDiskMSnExp (or XCMSnExp) object.

Usage

```
## S4 method for signature 'OnDiskMSnExp'
dirname(path)

## S4 replacement method for signature 'OnDiskMSnExp'
dirname(path) <- value
```

Arguments

path	OnDiskMSnExp.
value	character of length 1 or length equal to the number of files defining the new path to the files.

Author(s)

Johannes Rainer

---

doubleMatrix *Allocate double, integer, or logical matricies*

Description

Allocate double, integer, or logical matricies in one step without copying memory around.

Usage

```
doubleMatrix(nrow = 0, ncol = 0)
integerMatrix(nrow = 0, ncol = 0)
logicalMatrix(nrow = 0, ncol = 0)
```

Arguments

nrow	number of matrix rows
ncol	number of matrix columns

Value

Matrix of double, integer, or logical values. Memory is not zeroed.

Author(s)

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

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

Description

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

Usage

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

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` For `PeakGroupsParam`: `numeric(1)` between 0 and 1 defining the minimum required proportion 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. Note that if `subset` is provided, the specified fraction is relative to the defined subset of samples and not to the total number of samples within the experiment (i.e., a peak has to be present in the specified proportion of subset samples).

`extraPeaks` For `PeakGroupsParam`: `numeric(1)` defining the maximal number of additional peaks for all samples to be assigned to a peak group (feature) for retention time correction. For a data set with 6 samples, `extraPeaks = 1` uses all peak groups with a total peak count `<= 6 + 1`. The total peak count is the total number of peaks being assigned to a peak group and considers also multiple peaks within a sample that are assigned to the group.

`smooth` For `PeakGroupsParam`: `character(1)` defining the function to be used to interpolate corrected retention times for all peak groups. Can be either `"loess"` or `"linear"`.

`span` For `PeakGroupsParam`: `numeric(1)` defining the degree of smoothing (if `smooth = "loess"`). This parameter is passed to the internal call to `loess()`.

`family` For `PeakGroupsParam`: `character(1)` defining the method 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.

`subset` For `ObiwarpParam` and `PeakGroupsParam`: `integer` with the indices of samples within the experiment on which the alignment models should be estimated. Samples not part of the subset are adjusted based on the closest subset sample. See *Subset-based alignment* section for details.

`subsetAdjust` For `ObiwarpParam` and `PeakGroupsParam`: `character(1)` specifying the method with which non-subset samples should be adjusted. Supported options are `"previous"` and `"average"` (default). See *Subset-based alignment* section for details.

Details

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

Parameter `subset` allows to define a subset of samples within the experiment that should be aligned. All samples not being part of the subset will be aligned based on the adjustment of the closest sample

within the subset. This allows to e.g. exclude blank samples from the alignment process with their retention times being still adjusted based on the alignment results of the *real* samples.

Value

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

Note

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

Author(s)

Colin Smith, Johannes Rainer

References

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

`do_findChromPeaks_centWave`

Core API function for centWave peak detection

Description

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

Usage

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

```
  roiList = list(),
  firstBaselineCheck = TRUE,
  roiScales = NULL,
  sleep = 0,
  extendLengthMSW = FALSE,
  verboseBetaColumns = FALSE
)
```

Arguments

mz	Numeric vector with the individual m/z values from all scans/ spectra of one file/sample.
int	Numeric vector with the individual intensity values from all scans/spectra of one file/sample.
scantime	Numeric vector of length equal to the number of spectra/scans of the data representing the retention time of each scan.
valsPerSpect	Numeric vector with the number of values for each spectrum.
ppm	numeric(1) defining the maximal tolerated m/z deviation in consecutive scans in parts per million (ppm) for the initial ROI definition.
peakwidth	numeric(2) with the expected approximate peak width in chromatographic space. Given as a range (min, max) in seconds.
snthresh	numeric(1) defining the signal to noise ratio cutoff.
prefilter	numeric(2): c(k, I) specifying the prefilter step for the first analysis step (ROI detection). Mass traces are only retained if they contain at least k peaks with intensity >= I.
mzCenterFun	Name of the function to calculate the m/z center of the chromatographic peak. Allowed are: "wMean": intensity weighted mean of the peak's m/z values, "mean": mean of the peak's m/z values, "apex": use the m/z value at the peak apex, "wMeanApex3": intensity weighted mean of the m/z value at the peak apex and the m/z values left and right of it and "meanApex3": mean of the m/z value of the peak apex and the m/z values left and right of it.
integrate	Integration method. For integrate = 1 peak limits are found through descent on the mexican hat filtered data, for integrate = 2 the descent is done on the real data. The latter method is more accurate but prone to noise, while the former is more robust, but less exact.
mzdiff	numeric(1) representing the minimum difference in m/z dimension 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. In detail, a first rough estimate of the noise is calculated and peak detection is performed only in regions in which multiple sequential signals are higher than this first estimated baseline/noise level.

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

`sleep` `numeric(1)` defining the number of seconds to wait between iterations. Defaults to `sleep = 0`. If `> 0` a plot is generated visualizing the identified chromatographic peak. Note: this argument is for backward compatibility only and will be removed in future.

`extendLengthMSW`
Option to force centWave to use all scales when running centWave rather than truncating with the EIC length. Uses the "open" method to extend the EIC to a integer base-2 length prior to being passed to `convolve` rather than the default "reflect" method. See https://github.com/sneumann/xcms/issues/445 for more information.

`verboseBetaColumns`
Option to calculate two additional metrics of peak quality via comparison to an idealized bell curve. Adds `beta_cor` and `beta_snr` to the `chromPeaks` output, corresponding to a Pearson correlation coefficient to a bell curve with several degrees of skew as well as an estimate of signal-to-noise using the residuals from the best-fitting bell curve. See https://github.com/sneumann/xcms/pull/685 and https://doi.org/10.1186/s12859-023-05533-4 for more information.

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 `(maxo - baseline)/sd`, `sd` being the standard deviation of local chromatographic noise.

egauss RMSE of Gaussian fit.

Additional columns for `verboseColumns = TRUE`:

mu Gaussian parameter mu.

sigma Gaussian parameter sigma.

h Gaussian parameter h.

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

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

scale Scale on which the peak was localized.

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

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

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

Additional columns for `verboseBetaColumns = TRUE`:

beta_cor Correlation between an "ideal" bell curve and the raw data

beta_snr Signal-to-noise residuals calculated from the beta_cor fit

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_massifqu
do_findChromPeaks_matchedFilter(), do_findPeaks_MSW()

Examples

```
## Load the test file
faahko_sub <- loadXcmsData("faahko_sub")

## Subset to one file and restrict to a certain retention time range
data <- filterRt(filterFile(faahko_sub, 1), c(2500, 3000))

## Get m/z and intensity values
mzs <- mz(data)
ints <- intensity(data)

## Define the values per spectrum:
valsPerSpect <- lengths(mzs)

## Calling the function. We're using a large value for noise and prefilter
## to speed up the call in the example - 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 = unlist(mzs), int = unlist(ints),
    scantime = rtime(data), valsPerSpect = valsPerSpect, noise = 10000,
    prefilter = c(3, 10000))
head(res)
```

---

do_findChromPeaks_centWaveWithPredIsoROIs

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

---

Description

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

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

Usage

```
do_findChromPeaks_centWaveWithPredIsoROIs(
  mz,
  int,
  scantime,
  valsPerSpect,
  ppm = 25,
  peakwidth = c(20, 50),
  snthresh = 10,
  prefilter = c(3, 100),
  mzCenterFun = "wMean",
  integrate = 1,
  mzdiff = -0.001,
  fitgauss = FALSE,
  noise = 0,
  verboseColumns = FALSE,
  roiList = list(),
  firstBaselineCheck = TRUE,
  roiScales = NULL,
  snthreshIsoROIs = 6.25,
  maxCharge = 3,
  maxIso = 5,
  mzIntervalExtension = TRUE,
  polarity = "unknown",
  extendLengthMSW = FALSE,
  verboseBetaColumns = FALSE
)

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

)

Arguments

mz	Numeric vector with the individual m/z values from all scans/ spectra of one file/sample.
int	Numeric vector with the individual intensity values from all scans/spectra of one file/sample.
scantime	Numeric vector of length equal to the number of spectra/scans of the data representing the retention time of each scan.
valsPerSpect	Numeric vector with the number of values for each spectrum.
ppm	numeric(1) defining the maximal tolerated m/z deviation in consecutive scans in parts per million (ppm) for the initial ROI definition.
peakwidth	numeric(2) with the expected approximate peak width in chromatographic space. Given as a range (min, max) in seconds.
snthresh	For do_findChromPeaks_addPredIsoROIs: numeric(1) defining the signal to noise threshold for the centWave algorithm. For do_findChromPeaks_centWaveWithPredIsoROIs: numeric(1) defining the signal to noise threshold for the initial (first) centWave run.
prefilter	numeric(2): c(k, I) specifying the prefilter step for the first analysis step (ROI detection). Mass traces are only retained if they contain at least k peaks with intensity >= I.
mzCenterFun	Name of the function to calculate the m/z center of the chromatographic peak. Allowed are: "wMean": intensity weighted mean of the peak's m/z values, "mean": mean of the peak's m/z values, "apex": use the m/z value at the peak apex, "wMeanApex3": intensity weighted mean of the m/z value at the peak apex and the m/z values left and right of it and "meanApex3": mean of the m/z value of the peak apex and the m/z values left and right of it.
integrate	Integration method. For integrate = 1 peak limits are found through descent on the mexican hat filtered data, for integrate = 2 the descent is done on the real data. The latter method is more accurate but prone to noise, while the former is more robust, but less exact.
mzdiff	numeric(1) representing the minimum difference in m/z dimension 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. In detail, a first rough estimate of the noise is calculated and peak detection is performed only in regions in which multiple sequential signals are higher than this first estimated baseline/noise level.

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

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

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

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

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

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

`extendLengthMSW`
: Option to force centWave to use all scales when running centWave rather than truncating with the EIC length. Uses the "open" method to extend the EIC to a integer base-2 length prior to being passed to `convolve` rather than the default "reflect" method. See https://github.com/sneumann/xcms/issues/445 for more information.

`verboseBetaColumns`
: Option to calculate two additional metrics of peak quality via comparison to an idealized bell curve. Adds `beta_cor` and `beta_snr` to the `chromPeaks` output, corresponding to a Pearson correlation coefficient to a bell curve with several degrees of skew as well as an estimate of signal-to-noise using the residuals from the best-fitting bell curve. See https://github.com/sneumann/xcms/pull/685 and https://doi.org/10.1186/s12859-023-05533-4 for more information.

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

Details

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

Value

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

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

mzmin Minimum m/z of the peaks.

mzmax Maximum m/z of the peaks.

rt Retention time of the peak's midpoint.

rtmin Minimum retention time of the peak.

rtmax Maximum retention time of the peak.

into Integrated (original) intensity of the peak.

intb Per-peak baseline corrected integrated peak intensity.

maxo Maximum intensity of the peak.

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

egauss RMSE of Gaussian fit.

Additional columns for `verboseColumns = TRUE`:

mu Gaussian parameter mu.

sigma Gaussian parameter sigma.

h Gaussian parameter h.

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

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

scale Scale on which the peak was localized.

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

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

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

Additional columns for `verboseBetaColumns = TRUE`:

beta_cor Correlation between an "ideal" bell curve and the raw data

beta_snr Signal-to-noise residuals calculated from the beta_cor fit

Author(s)

Hendrik Treutler, Johannes Rainer

See Also

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

do_findChromPeaks_massifquant *Core API function for massifquant peak detection*

Description

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

Usage

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

Arguments

mz	Numeric vector with the individual m/z values from all scans/ spectra of one file/sample.
int	Numeric vector with the individual intensity values from all scans/spectra of one file/sample.
scantime	Numeric vector of length equal to the number of spectra/scans of the data representing the retention time of each scan.
valsPerSpect	Numeric vector with the number of values for each spectrum.
ppm	numeric(1) defining the maximal tolerated m/z deviation in consecutive scans in parts per million (ppm) for the initial ROI definition.

peakwidth numeric(2) with the expected approximate peak width in chromatographic space. Given as a range (min, max) in seconds.

snthresh numeric(1) defining the signal to noise ratio cutoff.

prefilter numeric(2): c(k, I) specifying the prefilter step for the first analysis step (ROI detection). Mass traces are only retained if they contain at least k peaks with intensity >= I.

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

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

mzdiff numeric(1) representing the minimum difference in m/z dimension 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 prediciton margin of error. A real centroid belonging to a bonafide peak must fall within the KF prediction margin of error. Much like in the construction of a confidence interval, criticalVal loosely translates to be a multiplier of the standard error of the prediction reported by the Kalman Filter. If the peak in the XC-MS sample have a small mass deviance in ppm error, a smaller critical value might be better and vice versa.

consecMissedLimit

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

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

(merges them) into one with a two sample t-test. The potential danger of this option is that some truly distinct peaks may be merged.

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

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

Details

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

Value

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

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

mzmin Minumum m/z of the peak.

mzmax Maximum m/z of the peak.

rtmin Minimum retention time of the peak.

rtmax Maximum retention time of the peak.

rt Retention time of the peak's midpoint.

into Integrated (original) intensity of the peak.

maxo Maximum intensity of the peak.

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

Author(s)

Christopher Conley

References

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

See Also

`massifquant` for the standard user interface method.

Other core peak detection functions: `do_findChromPeaks_centWave()`, `do_findChromPeaks_centWaveWithPredIsoROIs` `do_findChromPeaks_matchedFilter()`, `do_findPeaks_MSW()`

Examples

```
## Load the test file
faahko_sub <- loadXcmsData("faahko_sub")

## Subset to one file and restrict to a certain retention time range
data <- filterRt(filterFile(faahko_sub, 1), c(2500, 3000))

## Get m/z and intensity values
mzs <- mz(data)
ints <- intensity(data)

## Define the values per spectrum:
valsPerSpect <- lengths(mzs)

## Perform the peak detection using massifquant - setting prefilter to
## a high value to speed up the call for the example
res <- do_findChromPeaks_massifquant(mz = unlist(mzs), int = unlist(ints),
    scantime = rtime(data), valsPerSpect = valsPerSpect,
    prefilter = c(3, 10000))
head(res)
```

`do_findChromPeaks_matchedFilter` *Core API function for matchedFilter peak detection*

Description

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

Usage

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

Arguments

mz	Numeric vector with the individual m/z values from all scans/ spectra of one file/sample.
int	Numeric vector with the individual intensity values from all scans/spectra of one file/sample.
scantime	Numeric vector of length equal to the number of spectra/scans of the data representing the retention time of each scan.
valsPerSpect	Numeric vector with the number of values for each spectrum.
binSize	numeric(1) specifying the width of the bins/slices in m/z dimension.
impute	Character string specifying the method to be used for missing value imputation. Allowed values are "none" (no linear interpolation), "lin" (linear interpolation), "linbase" (linear interpolation within a certain bin-neighborhood) and "intlin". See imputeLinInterpol for more details.
baseValue	The base value to which empty elements should be set. This is only considered for method = "linbase" and corresponds to the profBinLinBase's baselevel argument.
distance	For method = "linbase": number of non-empty neighboring element of an empty element that should be considered for linear interpolation. See details section for more information.
fwhm	numeric(1) specifying the full width at half maximum of matched filtration gaussian model peak. Only used to calculate the actual sigma, see below.
sigma	numeric(1) specifying the standard deviation (width) of the matched filtration model peak.
max	numeric(1) representing the maximum number of peaks that are expected/will be identified per slice.

snthresh	numeric(1) defining the signal to noise ratio cutoff.
steps	numeric(1) defining the number of bins to be merged before filtration (i.e. the number of neighboring bins that will be joined to the slice in which filtration and peak detection will be performed).
mzdiff	numeric(1) representing the minimum difference in m/z dimension 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 indicies should be returned instead of values for m/z and retention times.
sleep	numeric(1) defining the number of seconds to wait between iterations. Defaults to sleep = 0. If > 0 a plot is generated visualizing the identified chromatographic peak. Note: this argument is for backward compatibility only and will be removed in future.

Details

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

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

Value

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

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

mzmin Minimum m/z of the peak.

mzmax Maximum m/z of the peak.

rt Retention time of the peak's midpoint.

rtmin Minimum retention time of the peak.

rtmax Maximum retention time of the peak.

into Integrated (original) intensity of the peak.

intf Integrated intensity of the filtered peak.

maxo Maximum intensity of the peak.

maxf Maximum intensity of the filtered peak.

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

sn Signal to noise ratio of the peak

Note

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

Author(s)

Colin A Smith, Johannes Rainer

References

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

See Also

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

Other core peak detection functions: do_findChromPeaks_centWave(), do_findChromPeaks_centWaveWithPredIsoROIs do_findChromPeaks_massifquant(), do_findPeaks_MSW()

Examples

```
## Load the test file
faahko_sub <- loadXcmsData("faahko_sub")

## Subset to one file and restrict to a certain retention time range
data <- filterRt(filterFile(faahko_sub, 1), c(2500, 3000))

## Get m/z and intensity values
mzs <- mz(data)
ints <- intensity(data)

## Define the values per spectrum:
valsPerSpect <- lengths(mzs)

res <- do_findChromPeaks_matchedFilter(mz = unlist(mzs), int = unlist(ints),
    scantime = rtime(data), 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,
  scantime = numeric(),
  valsPerSpect = integer(),
  ...
)
```

Arguments

mz	Numeric vector with the individual m/z values from all scans/ spectra of one file/sample.
int	Numeric vector with the individual intensity values from all scans/spectra of one file/sample.
snthresh	numeric(1) defining the signal to noise ratio cutoff.
verboseColumns	logical(1) whether additional peak meta data columns should be returned.
scantime	ignored.
valsPerSpect	ignored.
...	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_centWave(), do_findChromPeaks_centWaveWithPredIsoROIs 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. By default (with parameter ppm = 0) these m/z ranges have all the same (constant) size (depending on parameter binSize). For values of ppm larger than 0 the m/z bins (ranges or slices) will have increasing sizes depending on the m/z value. This better models the m/z-dependent measurement error/precision seen on some MS instruments.

Usage

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

Arguments

peaks	A matrix or data.frame with the mz values and retention times of the identified chromatographic peaks in all samples of an experiment. Required columns are "mz", "rt" and "sample". The latter should contain numeric values representing the index of the sample in which the peak was found.

sampleGroups	For PeakDensityParam: A vector of the same length than samples defining the sample group assignments (i.e. which samples belong to which sample group). This parameter is mandatory for the PeakDensityParam and has to be provided also if there is no sample grouping in the experiment (in which case all samples should be assigned to the same group).
bw	For PeakDensityParam: numeric(1) defining the bandwidth (standard deviation ot the smoothing kernel) to be used. This argument is passed to the [density() method.
minFraction	For PeakDensityParam: 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	For PeakDensityParam: 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	For PeakDensityParam: numeric(1) defining the size of the overlapping slices in m/z dimension.
maxFeatures	For PeakDensityParam: numeric(1) with the maximum number of peak groups to be identified in a single mz slice.
sleep	numeric(1) defining the time to *sleep* between iterations and plot the result from the current iteration.
index	An optional integer providing the indices of the peaks in the original peak matrix.
ppm	For MzClustParam: numeric(1) representing the relative m/z error for the clustering/grouping (in parts per million). For PeakDensityParam: numeric(1) to define m/z-dependent, increasing m/z bin sizes. If ppm = 0 (the default) m/z bins are defined by the sequence of values from the smallest to the larges m/z value with a constant bin size of binSize. For ppm > 0 the size of each bin is increased in addition by the ppm of the (upper) m/z boundary of the bin. The maximal bin size (used for the largest m/z values) would then be binSize plus ppm parts-per-million of the largest m/z value of all peaks in the data set.

Details

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

Value

A data.frame, 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.
- "peakidx": a list with the indices of all peaks in a feature in the peaks input matrix.

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.

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 file
library(xcms)
library(MsExperiment)
faahko_sub <- loadXcmsData("faahko_sub2")

## Disable parallel processing for this example
register(SerialParam())

## Extract the matrix with the identified peaks from the xcmsSet:
pks <- chromPeaks(faahko_sub)

## Perform the peak grouping with default settings:
res <- do_groupChromPeaks_density(pks, sampleGroups = rep(1, 3))

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

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

Description

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

Usage

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

Arguments

`peaks`	A `matrix` or `data.frame` with the mz values and retention times of the identified chromatographic peaks in all samples of an experiment. Required columns are `"mz"`, `"rt"` and `"sample"`. The latter should contain `numeric` values representing the index of the sample in which the peak was found.
`sampleGroups`	For `PeakDensityParam`: A vector of the same length than samples defining the sample group assignments (i.e. which samples belong to which sample group). This parameter is mandatory for the `PeakDensityParam` and has to be provided also if there is no sample grouping in the experiment (in which case all samples should be assigned to the same group).
`mzVsRtBalance`	For `NearestPeaksParam`: `numeric(1)` representing the factor by which m/z values are multiplied before calculating the (euclician) distance between two peaks.
`absMz`	For `NearestPeaksParam` and `MzClustParam`: `numeric(1)` maximum tolerated distance for m/z values.
`absRt`	For `NearestPeaksParam`: `numeric(1)` maximum tolerated distance for retention times.
`kNN`	For `NearestPeaksParam`: `integer(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	For PeakDensityParam: 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	For MzClustParam: numeric(1) representing the relative m/z error for the clustering/grouping (in parts per million). For PeakDensityParam: numeric(1) to define m/z-dependent, increasing m/z bin sizes. If ppm = 0 (the default) m/z bins are defined by the sequence of values from the smallest to the larges m/z value with a constant bin size of binSize. For ppm > 0 the size of each bin is increased in addition by the ppm of the (upper) m/z boundary of the bin. The maximal bin size (used for the largest m/z values) would then be binSize plus ppm parts-per-million of the largest m/z value of all peaks in the data set.
absMz	For NearestPeaksParam and MzClustParam: numeric(1) maximum tolerated distance for m/z values.
minFraction	For PeakDensityParam: 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	For PeakDensityParam: 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()`

`DratioFilter` *Filter features based on the dispersion ratio*

Description

The 'DratioFilter' class and method enable users to filter features from an 'XcmsExperiment' or 'SummarizedExperiment' object based on the D-ratio or *dispersion ratio*. This is defined as the standard deviation for QC samples divided by the standard deviation for biological test samples, for each feature of the object (Broadhurst et al.).

This 'filter' is part of the possible dispatch of the generic function 'filterFeatures'. Features *above* ('>') the user-input threshold will be removed from the entire dataset.

Usage

```
DratioFilter(
  threshold = 0.5,
  qcIndex = integer(),
  studyIndex = integer(),
  na.rm = TRUE,
  mad = FALSE
)

## S4 method for signature 'XcmsResult,DratioFilter'
filterFeatures(object, filter, ...)

## S4 method for signature 'SummarizedExperiment,DratioFilter'
filterFeatures(object, filter, assay = 1)
```

Arguments

`threshold`	'numeric' value representing the threshold. Features with a D-ratio *strictly higher* ('>') than this will be removed from the entire dataset.
`qcIndex`	'integer' (or 'logical') vector corresponding to the indices of QC samples.
`studyIndex`	'integer' (or 'logical') vector corresponding of the indices of study samples.
`na.rm`	'logical' Indicates whether missing values ('NA') should be removed prior to the calculations.

mad	'logical' Indicates whether the *Median Absolute Deviation* (MAD) should be used instead of the standard deviation. This is suggested for non-gaussian distributed data.
object	XcmsExperiment or SummarizedExperiment. For an XcmsExperiment object, the featureValues(object) will be evaluated, and for Summarizedesxperiment the assay(object, assay). The object will be filtered.
filter	The parameter object selecting and configuring the type of filtering. It can be one of the following classes: RsdFilter, DratioFilter, PercentMissingFilter or BlankFlag.
...	Optional parameters. For object being an XcmsExperiment: parameters for the featureValues() call.
assay	For filtering of SummarizedExperiment objects only. Indicates which assay the filtering will be based on. Note that the features for the entire object will be removed, but the computations are performed on a single assay. Default is 1, which means the first assay of the object will be evaluated.

Value

For 'DratioFilter': a 'DratioFilter' class. 'filterFeatures' return the input object minus the features that did not met the user input threshold

Author(s)

Philippine Louail

References

Broadhurst D, Goodacre R, Reinke SN, Kuligowski J, Wilson ID, Lewis MR, Dunn WB. Guidelines and considerations for the use of system suitability and quality control samples in mass spectrometry assays applied in untargeted clinical metabolomic studies. Metabolomics. 2018;14(6):72. doi: 10.1007/s11306-018-1367-3. Epub 2018 May 18. PMID: 29805336; PMCID: PMC5960010.

See Also

Other Filter features in xcms: BlankFlag, PercentMissingFilter, RsdFilter

---

`estimatePrecursorIntensity`

Estimate precursor intensity for MS level 2 spectra

Description

estimatePrecursorIntensity determines the precursor intensity for a MS 2 spectrum based on the intensity of the respective signal from the neighboring MS 1 spectra (i.e. based on the peak with the m/z matching the precursor m/z of the MS 2 spectrum). Based on parameter method either the intensity of the peak from the previous MS 1 scan is used (method = "previous") or an interpolation between the intensity from the previous and subsequent MS1 scan is used (method = "interpolation", which considers also the retention times of the two MS1 scans and the retention time of the MS2 spectrum).

Usage

```
estimatePrecursorIntensity(
  x,
  ppm = 10,
  method = c("previous", "interpolation"),
  BPPARAM = bpparam()
)
```

Arguments

x	OnDiskMSnExp or XCMSnExp object.
ppm	numeric(1) defining the maximal acceptable difference (in ppm) of the precursor m/z and the m/z of the corresponding peak in the MS 1 scan.
method	character(1) defining the method how the precursor intensity should be determined (see description above for details). Defaults to method = "previous".
BPPARAM	parallel processing setup. See bpparam() for details.

Value

numeric with length equal to the number of spectra in x. NA is returned for MS 1 spectra or if no matching peak in a MS 1 scan can be found for an MS 2 spectrum

Author(s)

Johannes Rainer

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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

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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,
  groupnames = FALSE,
  ...
)
```

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 getOption("digits"). See format() for more information.
groupnames	logical(1) whether row names of the resulting matrix should be the feature IDs (groupnames = FALSE; default) or IDs that are composed of the m/z and retention time of the features (in the format M<m/z>T<rt> (groupnames = TRUE). See help of the groupnames function for details.
...	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

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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

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

Value

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

Author(s)

Johannes Rainer

See Also

XCMSnExp for the data object.

Examples

```
## Load a test data set with detected peaks
library(MSnbase)
data(faahko_sub)
## Update the path to the files for the local system
dirname(faahko_sub) <- system.file("cdf/KO", package = "faahKO")

## Disable parallel processing for this example
```

```
register(SerialParam())

## Extract the full MS data for a certain retention time range
## as a data.frame
tmp <- filterRt(faahko_sub, rt = c(2800, 2900))
ms_all <- as(tmp, "data.frame")
head(ms_all)
nrow(ms_all)
```

---

feature-grouping *Compounding of LC-MS features*

Description

Feature *compounding* aims at identifying and grouping LC-MS features representing different ions or adducts (including isotopes) of the same originating compound. The MsFeatures package provides a general framework and functionality to group features based on different properties. The `groupFeatures` methods for `XcmsExperiment()` or XCMSnExp objects implemented in `xcms` extend these to enable the *compounding* of LC-MS data considering also e.g. feature peak shaped. Note that these functions simply define feature groups but don't actually *aggregate* or combine the features.

See `MsFeatures::groupFeatures()` for an overview on the general feature grouping concept as well as details on the individual settings and parameters.

The available options for `groupFeatures` on `xcms` preprocessing results (i.e. on `XcmsExperiment` or `XCMSnExp` objects after correspondence analysis with `groupChromPeaks()`) are:

- Grouping by similar retention times: `groupFeatures-similar-rtime()`.
- Grouping by similar feature values across samples: `AbundanceSimilarityParam()`.
- Grouping by similar peak shape of extracted ion chromatograms: `EicSimilarityParam()`.

An ideal workflow grouping features should sequentially perform the above methods (in the listed order).

Compounded feature groups can be accessed with the `featureGroups` function.

Usage

```
## S4 method for signature 'XcmsResult'
featureGroups(object)

## S4 replacement method for signature 'XcmsResult'
featureGroups(object) <- value
```

Arguments

`object`	an `XcmsExperiment()` or `XCMSnExp()` object with LC-MS pre-processing results.
`value`	for `featureGroups<-`: replacement for the feature groups in `object`. Has to be of length 1 or length equal to the number of features in `object`.

Author(s)

Johannes Rainer, Mar Garcia-Aloy, Vinicius Veri Hernandes

See Also

`plotFeatureGroups()` for visualization of grouped features.

`featureChromatograms` *Extract ion chromatograms for each feature*

Description

Extract ion chromatograms for features in an XcmsExperiment or XCMSnExp object. The function returns for each feature the extracted ion chromatograms (along with all associated chromatographic peaks) in each sample. The chromatogram is extracted from the m/z - rt region that includes **all** chromatographic peaks of a feature. By default, this region is defined using the range of the chromatographic peaks' m/z and retention times (with `mzmin = min`, `mzmax = max`, `rtmin = min` and `rtmax = max`). For some features, and depending on the data, the m/z and rt range can thus be relatively large. The boundaries of the m/z - rt region can also be restricted by changing parameters `mzmin`, `mzmax`, `rtmin` and `rtmax` to a different functions, such as `median`.

By default only chromatographic peaks associated with a feature are included in the returned XChromatograms object. For `object` being an `XCMSnExp` object parameter `include` allows also to return all chromatographic peaks with their apex position within the selected region (`include = "apex_within"`) or any chromatographic peak overlapping the m/z and retention time range (`include = "any"`).

Usage

```
featureChromatograms(object, ...)

## S4 method for signature 'XcmsExperiment'
featureChromatograms(
  object,
  expandRt = 0,
  expandMz = 0,
  aggregationFun = "max",
  features = character(),
  return.type = "XChromatograms",
  chunkSize = 2L,
  mzmin = min,
  mzmax = max,
  rtmin = min,
  rtmax = max,
  ...,
  progressbar = TRUE,
  BPPARAM = bpparam()
```

```
)

## S4 method for signature 'XCMSnExp'
featureChromatograms(
  object,
  expandRt = 0,
  aggregationFun = "max",
  features,
  include = c("feature_only", "apex_within", "any", "all"),
  filled = FALSE,
  n = length(fileNames(object)),
  value = c("maxo", "into"),
  expandMz = 0,
  ...
)
```

Arguments

object	XcmsExperiment or XCMSnExp object with grouped chromatographic peaks.
...	optional arguments to be passed along to the chromatogram() function.
expandRt	numeric(1) to expand the retention time range for each chromatographic peak by a constant value on each side.
expandMz	numeric(1) to expand the m/z range for each chromatographic peak by a constant value on each side. Be aware that by extending the m/z range the extracted EIC might **no longer** represent the actual identified chromatographic peak because intensities of potential additional mass peaks within each spectra would be aggregated into the final reported intensity value per spectrum (retention time).
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 "max" 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.
return.type	character(1) defining how the result should be returned. At present only return.type = "XChromatograms" is supported and the results are thus returned as an XChromatograms() object.
chunkSize	For object being an XcmsExperiment: integer(1) defining the number of files from which the data should be loaded at a time into memory. Defaults to chunkSize = 2L.
mzmin	function defining how the lower boundary of the m/z region from which the EIC is integrated should be defined. Defaults to mzmin = min thus the smallest "mzmin" value for all chromatographic peaks of a feature will be used.
mzmax	function defining how the upper boundary of the m/z region from which the EIC is integrated should be defined. Defaults to mzmax = max thus the largest "mzmax" value for all chromatographic peaks of a feature will be used.

rtmin	function defining how the lower boundary of the rt region from which the EIC is integrated should be defined. Defaults to rtmin = min thus the smallest "rtmin" value for all chromatographic peaks of a feature will be used.
rtmax	function defining how the upper boundary of the rt region from which the EIC is integrated should be defined. Defaults to rtmax = max thus the largest "rtmax" value for all chromatographic peaks of a feature will be used.
progressbar	logical(1) defining whether a progress bar is shown.
BPPARAM	For object being an XcmsExperiment: parallel processing setup. Defaults to BPPARAM = bpparam(). See bpparam() for more information.
include	Only for object being an XCMSnExp: character(1) defining which chromatographic peaks (and related feature definitions) should be included in the returned XChromatograms(). Defaults to "feature_only"; See description above for options and details.
filled	Only for object being an XCMSnExp: logical(1) whether filled-in peaks should be included in the result object. The default is filled = FALSE, i.e. only detected peaks are reported.
n	Only for object being an XCMSnExp: integer(1) to optionally specify the number of *top n* samples from which the EIC should be extracted.
value	Only for object being an XCMSnExp: character(1) specifying the column to be used to sort the samples. Can be either "maxo" (the default) or "into" to use the maximal peak intensity or the integrated peak area, respectively.

Value

XChromatograms() object. In future, depending on parameter return.type, the data might be returned as a different object.

Note

The EIC data of a feature is extracted from every sample using the same m/z - rt area. The EIC in a sample does thus not exactly represent the signal of the actually identified chromatographic peak in that sample. The chromPeakChromatograms() function would allow to extract the actual EIC of the chromatographic peak in a specific sample. See also examples below.

Parameters include, filled, n and value are only supported for object being an XCMSnExp.

When extracting EICs from only the top n samples it can happen that one or more of the features specified with features are dropped because they have no detected peak in the *top n* samples. The chance for this to happen is smaller if x contains also filled-in peaks (with fillChromPeaks).

Author(s)

Johannes Rainer

See Also

filterColumnsKeepTop() to filter the extracted EICs keeping only the *top n* columns (samples) with the highest intensity. chromPeakChromatograms() for a function to extract an EIC for each chromatographic peak.

Examples

```
## Load a test data set with detected peaks
library(xcms)
library(MsExperiment)
faahko_sub <- loadXcmsData("faahko_sub2")

## Disable parallel processing for this example
register(SerialParam())

## Perform correspondence analysis
xdata <- groupChromPeaks(faahko_sub,
    param = PeakDensityParam(minFraction = 0.8, sampleGroups = rep(1, 3)))

## Get the feature definitions
featureDefinitions(xdata)

## Extract ion chromatograms for the first 3 features. Parameter
## `features` can be either the feature IDs or feature indices.
chrs <- featureChromatograms(xdata,
    features = rownames(featureDefinitions)[1:3])

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

## The EICs for all 3 samples use the same m/z and retention time range,
## which was defined using the `featureArea` function:
featureArea(xdata, features = rownames(featureDefinitions(xdata))[1:3],
    mzmin = min, mzmax = max, rtmin = min, rtmax = max)

## To extract the actual (exact) EICs for each chromatographic peak of
## a feature in each sample, the `chromPeakChromatograms` function would
## need to be used instead. Below we extract the EICs for all
## chromatographic peaks of the first feature. We need to first get the
## IDs of all chromatographic peaks assigned to the first feature:
peak_ids <- rownames(chromPeaks(xdata))[featureDefinitions(xdata)$peakidx[[1L]]]

## We can now pass these to the `chromPeakChromatograms` function with
## parameter `peaks`:
eic_1 <- chromPeakChromatograms(xdata, peaks = peak_ids)

## To plot these into a single plot we need to use the
## `plotChromatogramsOverlay` function:
plotChromatogramsOverlay(eic_1)
```

---

featureSpectra *Extract spectra associated with features*

Description

This function returns spectra associated with the identified features in the input object. By default, spectra are returned for all features (from all MS levels), but parameter `features` allows to spec-

ify/select features for which the result should be returned. Parameter `msLevel` allows to define whether MS level 1 or 2 spectra should be returned. For `msLevel = 1L` all MS1 spectra within the retention time range of each chromatographic peak (in that respective data file) associated with a feature are returned. Note that for samples in which no peak was identified (or even filled-in) no spectra are returned. For `msLevel = 2L` all MS2 spectra with a retention time within the retention time range and their precursor m/z within the m/z range of any chromatographic peak of a feature are returned.

See also `chromPeakSpectra()` (used internally to extract spectra for each chromatographic peak of a feature) for additional information, specifically also on parameter `method`. By default (`method = "all"`) all spectra associated with any of the chromatographic peaks of a feature are returned. With any other option for `method`, a single spectrum **per chromatographic peak** will be returned (hence multiple spectra per feature).

The ID of each chromatographic peak (i.e. its row name in `chromPeaks`) and each feature (i.e., its row name in `featureDefinitions`) are available in the returned `Spectra()` with spectra variables `"peak_id"` and `"feature_id"`, respectively.

Usage

```
featureSpectra(object, ...)

## S4 method for signature 'XcmsExperiment'
featureSpectra(
  object,
  msLevel = 2L,
  expandRt = 0,
  expandMz = 0,
  ppm = 0,
  skipFilled = FALSE,
  return.type = c("Spectra", "List"),
  features = character(),
  ...
)

## S4 method for signature 'XCMSnExp'
featureSpectra(
  object,
  msLevel = 2L,
  expandRt = 0,
  expandMz = 0,
  ppm = 0,
  skipFilled = FALSE,
  return.type = c("MSpectra", "Spectra", "list", "List"),
  features = character(),
  ...
)
```

Arguments

object	XcmsExperiment or XCMSnExp object with feature defitions.
...	additional arguments to be passed along to chromPeakSpectra(), such as method.
msLevel	integer(1) defining the MS level of the spectra that should be returned.
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.
skipFilled	logical(1) whether spectra for filled-in peaks should be reported or not.
return.type	character(1) defining the type of result object that should be returned.
features	character, logical or integer allowing to specify a subset of features in featureDefinitions for which spectra should be returned (providing either their ID, a logical vector same length than nrow(featureDefinitions(x)) or their index in featureDefinitions(x)). This parameter overrides skipFilled and is only supported for return.type being either "Spectra" or "List".

Value

The function returns either a Spectra() (for return.type = "Spectra") or a List of Spectra (for return.type = "List"). For the latter, the order and the length matches parameter features (or if no features is defined the order of the features in featureDefinitions(object)).

Spectra variables "peak_id" and "feature_id" define to which chromatographic peak or feature each individual spectrum is associated with.

Author(s)

Johannes Rainer

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featureSummary *Simple feature summaries*

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	[XcmsExperiment()] or [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

fillChromPeaks *Gap Filling*

Description

Gap filling integrate signal in the m/z-rt area of a feature (i.e., a chromatographic peak group) for samples in which no chromatographic peak for this feature was identified and add it to the chromPeaks() matrix. Such *filled-in* peaks are indicated with a TRUE in column "is_filled" in the result object's chromPeakData() data frame.

The method for gap filling along with its settings can be defined with the param argument. Two different approaches are available:

- param = FillChromPeaksParam(): the default of the original xcms code. Signal is integrated from the m/z and retention time range as defined in the featureDefinitions() data frame, i.e. from the "rtmin", "rtmax", "mzmin" and "mzmax". This method is not suggested as it underestimates the actual peak area and it is also not available for object being an XcmsExperiment object. See details below for more information and settings for this method.
- param = ChromPeakAreaParam(): the area from which the signal for a feature is integrated is defined based on the feature's chromatographic peak areas. The m/z range is by default defined as the the lower quartile of chromatographic peaks' "mzmin" value to the upper quartile of the chromatographic peaks' "mzmax" values. The retention time range for the area is defined analogously. Alternatively, by setting mzmin = median, mzmax = median, rtmin = median and rtmax = median in ChromPeakAreaParam, the median "mzmin", "mzmax", "rtmin" and "rtmax" values from all detected chromatographic peaks of a feature would be used instead. In contrast to the FillChromPeaksParam approach this method uses (all) identified chromatographic peaks of a feature to define the area from which the signal should be integrated.

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.

Usage

```
fillChromPeaks(object, param, ...)

## S4 method for signature 'XcmsExperiment,ChromPeakAreaParam'
fillChromPeaks(
  object,
  param,
  msLevel = 1L,
  chunkSize = 2L,
  BPPARAM = bpparam()
)

FillChromPeaksParam(
  expandMz = 0,
```

```
  expandRt = 0,
  ppm = 0,
  fixedMz = 0,
  fixedRt = 0
)

fixedRt(object)

fixedMz(object)

ChromPeakAreaParam(
  mzmin = function(z) quantile(z, probs = 0.25, names = FALSE),
  mzmax = function(z) quantile(z, probs = 0.75, names = FALSE),
  rtmin = function(z) quantile(z, probs = 0.25, names = FALSE),
  rtmax = function(z) quantile(z, probs = 0.75, names = FALSE)
)

## 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, msLevel = 1L, BPPARAM = bpparam())

## S4 method for signature 'XCMSnExp,ChromPeakAreaParam'
fillChromPeaks(object, param, msLevel = 1L, BPPARAM = bpparam())

## S4 method for signature 'XCMSnExp,missing'
fillChromPeaks(object, param, BPPARAM = bpparam(), msLevel = 1L)
```

Arguments

object	XcmsExperiment or XCMSnExp object with identified and grouped chromatographic peaks.

param — ChromPeakAreaParam or FillChromPeaksParam object defining which approach should be used (see details section).

... — currently ignored.

msLevel — integer(1) defining the MS level on which peak filling should be performed (defaults to msLevel = 1L). Only peak filling on one MS level at a time is supported, to fill in peaks for MS level 1 and 2 run first using msLevel = 1 and then (on the returned result object) again with msLevel = 2.

chunkSize — For fillChromPeaks if object is an XcmsExperiment: integer(1) defining the number of files (samples) that should be loaded into memory and processed at the same time. This setting thus allows to balance between memory demand and speed (due to parallel processing). Because parallel processing can only performed on the subset of data currently loaded into memory in each iteration, the value for chunkSize should match the defined parallel setting setup. Using a parallel processing setup using 4 CPUs (separate processes) but using chunkSize = 1will not perform any parallel processing, as only the data from one sample i to the total number of samples in an experiment will load the full MS data into memory and will thus in most settings cause an out-of-memory error.

BPPARAM — Parallel processing settings.

expandMz — for FillChromPeaksParam: numeric(1) defining the value by which the mz width of peaks should be expanded. Each peak is expanded in mz direction by expandMz * their original m/z width. A value of 0 means no expansion, a value of 1 grows each peak by 1 * the m/z width of the peak resulting in peaks with twice their original size in m/z direction (expansion by half m/z width to both sides).

expandRt — for FillChromPeaksParam: numeric(1), same as expandMz but for the retention time width.

ppm — for FillChromPeaksParam: numeric(1) optionally specifying a *ppm* by which the m/z width of the peak region should be expanded. For peaks with an m/z width smaller than mean(c(mzmin, mzmax)) * ppm / 1e6, the mzmin will be replaced by mean(c(mzmin, mzmax)) - (mean(c(mzmin, mzmax)) * ppm / 2 / 1e6) mzmax by mean(c(mzmin, mzmax)) + (mean(c(mzmin, mzmax)) * ppm / 2 / 1e6). This is applied before eventually expanding the m/z width using the expandMz parameter.

fixedMz — for FillChromPeaksParam: 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 *after* expandMz and ppm.

fixedRt — for FillChromPeaksParam: 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 *after* expandRt.

mzmin — function to be applied to values in the "mzmin" column of all chromatographic peaks of a feature to define the lower m/z value of the area from which signal for the feature should be integrated. Defaults to mzmin = function(z) quantile(z, probs = 0.25) hence using the 25% quantile of all values.

mzmax — function to be applied to values in the "mzmax" column of all chromatographic peaks of a feature to define the upper m/z value of the area from which signal for the feature should be integrated. Defaults to mzmax = function(z) quantile(z, probs = 0.75) hence using the 75% quantile of all values.

rtmin — function to be applied to values in the "rtmin" column of all chromatographic peaks of a feature to define the lower rt value of the area from which signal for the feature should be integrated. Defaults to rtmin = function(z) quantile(z, probs = 0.25) hence using the 25% quantile of all values.

rtmax — function to be applied to values in the "rtmax" column of all chromatographic peaks of a feature to define the upper rt value of the area from which signal for the feature should be integrated. Defaults to rtmax = function(z) quantile(z, probs = 0.75) hence using the 75% quantile of all values.

value — The value for the slot.

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 m/z-rt region of the feature. Two different approaches to define this region are available: with ChromPeakAreaParam the region is defined based on the detected **chromatographic peaks** of a feature, while with FillChromPeaksParam the region is defined based on the m/z and retention times of the **feature** (which represent the m/z and retentention times of the apex position of the associated chromatographic peaks). For the latter approach various parameters are available to increase the area from which signal is to be integrated, 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 used 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 is used.

Value

An XcmsExperiment or XCMSnExp object with previously missing chromatographic peaks for features filled into its chromPeaks() matrix.

The FillChromPeaksParam function returns a FillChromPeaksParam object.

Slots

expandMz,expandRt,ppm,fixedMz,fixedRt See corresponding parameter above.

rtmin,rtmax,mzmin,mzmax See corresponding parameter above.

Note

The reported "mzmin", "mzmax", "rtmin" and "rtmax" for the filled peaks represents the actual MS area from which the signal was integrated.

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.

Author(s)

Johannes Rainer

See Also

groupChromPeaks() for methods to perform the correspondence.

featureArea for the function to define the m/z-retention time region for each feature.

Examples

```
## Load a test data set with identified chromatographic peaks
library(xcms)
library(MsExperiment)
res <- loadXcmsData("faahko_sub2")

## Disable parallel processing for this example
register(SerialParam())

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

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

## Filling missing peak data using the peak area from identified
## chromatographic peaks.
res <- fillChromPeaks(res, param = ChromPeakAreaParam())

## How many missing values do we have after peak filling?
sum(is.na(featureValues(res)))

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

## 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
```

```
## It is also possible to remove filled-in peaks:
res <- dropFilledChromPeaks(res)

sum(is.na(featureValues(res)))
```

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

Description

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

Arguments

`object`	the `xcmsSet` object
`method`	the filling method

Details

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

Value

A `xcmsSet` objects with filled in peak groups.

Methods

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

See Also

`xcmsSet-class`, `getPeaks`

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

Description

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

Arguments

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

Details

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

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

Value

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

Methods

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

See Also

xcmsSet-class, getPeaks fillPeaks

---

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

Description

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

Arguments

object	the xcmsSet object

Details

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

Value

A xcmsSet objects with filled in peak groups.

Methods

object = "xcmsSet" fillPeaks.MSW(object)

Note

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

See Also

xcmsSet-class, getPeaks fillPeaks

filterColumnsIntensityAbove,MChromatograms-method
Filtering sets of chromatographic data

Description

These functions allow to filter (subset) MChromatograms() or XChromatograms() objects, i.e. sets of chromatographic data, without changing the data (intensity and retention times) within the individual chromatograms (Chromatogram() objects).

- filterColumnsIntensityAbove: subsets a MChromatograms objects keeping only columns (samples) for which value is larger than the provided threshold in which rows (i.e. if which = "any" a column is kept if **any** of the chromatograms in that column have a value larger than threshold or with which = "all" **all** chromatograms in that column fulfill this criteria). Parameter value allows to define on which value the comparison should be performed, with value = "bpi" the maximum intensity of each chromatogram is compared to threshold, with value = "tic" the total sum of intensities of each chromatogram is compared to threshold. For XChromatogramsobject, value = "maxo"andvalue = "into"are supported which compares the largest i
or the integrated peak area, respectively.
- filterColumnsKeepTop: subsets a MChromatograms object keeping the top n columns sorted by the value specified with sortBy. In detail, for each column the value defined by sortBy is extracted from each chromatogram and aggregated using the aggregationFun. Thus, by default, for each chromatogram the maximum intensity is determined (sortBy = "bpi") and these values are summed up for chromatograms in the same column (aggregationFun = sum). The columns are then sorted by these values and the top n columns are retained in the returned MChromatograms. Similar to the filterColumnsIntensityAbove function, this function allows to use for XChromatograms objects to sort the columns by column sortBy = "maxo" or sortBy = "into" of the chromPeaks matrix.

Usage

```
## S4 method for signature 'MChromatograms'
filterColumnsIntensityAbove(
  object,
  threshold = 0,
  value = c("bpi", "tic"),
  which = c("any", "all")
)

## S4 method for signature 'MChromatograms'
filterColumnsKeepTop(
  object,
  n = 1L,
  sortBy = c("bpi", "tic"),
  aggregationFun = sum
)
```

```
## S4 method for signature 'XChromatograms'
filterColumnsIntensityAbove(
  object,
  threshold = 0,
  value = c("bpi", "tic", "maxo", "into"),
  which = c("any", "all")
)

## S4 method for signature 'XChromatograms'
filterColumnsKeepTop(
  object,
  n = 1L,
  sortBy = c("bpi", "tic", "maxo", "into"),
  aggregationFun = sum
)
```

Arguments

object	MChromatograms() or XChromatograms() object.
threshold	for filterColumnsIntensityAbove: numeric(1) with the threshold value to compare against.
value	character(1) defining which value should be used in the comparison or sorting. Can be value = "bpi" (default) to use the maximum intensity per chromatogram or value = "tic" to use the sum of intensities per chromatogram. For XChromatograms() objects also value = "maxo" and value = "into" is supported to use the maximum intensity or the integrated area of identified chromatographic peaks in each chromatogram.
which	for filterColumnsIntensityAbove: character(1) defining whether **any** (which = "any", default) or **all** (which = "all") chromatograms in a column have to fulfill the criteria for the column to be kept.
n	for filterColumnsKeepTop: integer(1) specifying the number of columns that should be returned. n will be rounded to the closest (larger) integer value.
sortBy	for filterColumnsKeepTop: the value by which columns should be ordered to determine the top n columns. Can be either sortBy = "bpi" (the default), in which case the maximum intensity of each column's chromatograms is used, or sortBy = "tic" to use the total intensity sum of all chromatograms. For XChromatograms() objects also value = "maxo" and value = "into" is supported to use the maximum intensity or the integrated area of identified chromatographic peaks in each chromatogram.
aggregationFun	for filterColumnsKeepTop: function to be used to aggregate (combine) the values from all chromatograms in each column. Defaults to aggregationFun = sum in which case the sum of the values is used to rank the columns. Alternatively the mean, median or similar function can be used.

Value

a filtered MChromatograms (or XChromatograms) object with the same number of rows (EICs) but eventually a lower number of columns (samples).

Author(s)

Johannes Rainer

Examples

```
library(MSnbase)
chr1 <- Chromatogram(rtime = 1:10 + rnorm(n = 10, sd = 0.3),
    intensity = c(5, 29, 50, NA, 100, 12, 3, 4, 1, 3))
chr2 <- Chromatogram(rtime = 1:10 + rnorm(n = 10, sd = 0.3),
    intensity = c(80, 50, 20, 10, 9, 4, 3, 4, 1, 3))
chr3 <- Chromatogram(rtime = 3:9 + rnorm(7, sd = 0.3),
    intensity = c(53, 80, 130, 15, 5, 3, 2))

chrs <- MChromatograms(list(chr1, chr2, chr1, chr3, chr2, chr3),
    ncol = 3, byrow = FALSE)
chrs

#### filterColumnsIntensityAbove
##
## Keep all columns with for which the maximum intensity of any of its
## chromatograms is larger 90
filterColumnsIntensityAbove(chrs, threshold = 90)

## Require that ALL chromatograms in a column have a value larger 90
filterColumnsIntensityAbove(chrs, threshold = 90, which = "all")

## If none of the columns fulfills the criteria no columns are returned
filterColumnsIntensityAbove(chrs, threshold = 900)

## Filtering XChromatograms allow in addition to filter on the columns
## "maxo" or "into" of the identified chromatographic peaks within each
## chromatogram.

#### filterColumnsKeepTop
##
## Keep the 2 columns with the highest sum of maximal intensities in their
## chromatograms
filterColumnsKeepTop(chrs, n = 1)

## Keep the 50 percent of columns with the highest total sum of signal. Note
## that n will be rounded to the next larger integer value
filterColumnsKeepTop(chrs, n = 0.5 * ncol(chrs), sortBy = "tic")
```

`filterFeatureDefinitions`

Next Generation `xcms` *Result Object*

Description

The XcmsExperiment is a data container for xcms preprocessing results (i.e. results from chromatographic peak detection, alignment and correspondence analysis).

It provides the same functionality than the XCMSnExp object, but uses the more advanced and modern MS infrastructure provided by the MsExperiment and Spectra Bioconductor packages. With this comes a higher flexibility on how and where to store the data.

Documentation of the various functions for XcmsExperiment objects are grouped by topic and provided in the sections below.

The default xcms workflow is to perform

- chromatographic peak detection using findChromPeaks()
- optionally refine identified chromatographic peaks using refineChromPeaks()
- perform an alignment (retention time adjustment) using adjustRtime(). Depending on the method used this requires to run a correspondence analysis first
- perform a correspondence analysis using the groupChromPeaks() function to group chromatographic peaks across samples to define the LC-MS features.
- optionally perform a gap-filling to *rescue* signal in samples in which no chromatographic peak was identified and hence a missing value would be reported. This can be performed using the fillChromPeaks() function.

Usage

```
filterFeatureDefinitions(object, ...)

## S4 method for signature 'MsExperiment'
filterRt(object, rt = numeric(), ...)

## S4 method for signature 'MsExperiment'
filterMzRange(object, mz = numeric(), msLevel. = uniqueMsLevels(object))

## S4 method for signature 'MsExperiment'
filterMz(object, mz = numeric(), msLevel. = uniqueMsLevels(object))

## S4 method for signature 'MsExperiment'
filterMsLevel(object, msLevel. = uniqueMsLevels(object))

## S4 method for signature 'MsExperiment'
uniqueMsLevels(object)

## S4 method for signature 'MsExperiment'
filterFile(object, file = integer(), ...)

## S4 method for signature 'MsExperiment'
rtime(object)

## S4 method for signature 'MsExperiment'
```

```
fromFile(object)

## S4 method for signature 'MsExperiment'
fileNames(object)

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

## S4 method for signature 'MsExperiment'
filterIsolationWindow(object, mz = numeric())

## S4 method for signature 'MsExperiment'
chromatogram(
  object,
  rt = matrix(nrow = 0, ncol = 2),
  mz = matrix(nrow = 0, ncol = 2),
  aggregationFun = "sum",
  msLevel = 1L,
  isolationWindowTargetMz = NULL,
  chunkSize = 2L,
  return.type = "MChromatograms",
  BPPARAM = bpparam()
)

## S4 method for signature 'XcmsExperiment,ANY,ANY,ANY'
x[i, j, ..., drop = TRUE]

## S4 method for signature 'XcmsExperiment'
filterIsolationWindow(object, mz = numeric())

## S4 method for signature 'XcmsExperiment'
filterRt(object, rt, msLevel.)

## S4 method for signature 'XcmsExperiment'
filterMzRange(object, mz = numeric(), msLevel. = uniqueMsLevels(object))

## S4 method for signature 'XcmsExperiment'
filterMsLevel(object, msLevel. = uniqueMsLevels(object))

## S4 method for signature 'XcmsExperiment'
hasChromPeaks(object, msLevel = integer())

## S4 method for signature 'XcmsExperiment'
dropChromPeaks(object, keepAdjustedRtime = FALSE)

## S4 replacement method for signature 'XcmsExperiment'
chromPeaks(object) <- value
```

```
## S4 method for signature 'XcmsExperiment'
chromPeaks(
  object,
  rt = numeric(),
  mz = numeric(),
  ppm = 0,
  msLevel = integer(),
  type = c("any", "within", "apex_within"),
  isFilledColumn = FALSE
)

## S4 replacement method for signature 'XcmsExperiment'
chromPeakData(object) <- value

## S4 method for signature 'XcmsExperiment'
chromPeakData(
  object,
  msLevel = integer(),
  return.type = c("DataFrame", "data.frame")
)

## S4 method for signature 'XcmsExperiment'
filterChromPeaks(
  object,
  keep = rep(TRUE, nrow(.chromPeaks(object))),
  method = "keep",
  ...
)

## S4 method for signature 'XcmsExperiment'
dropAdjustedRtime(object)

## S4 method for signature 'MsExperiment'
hasAdjustedRtime(object)

## S4 method for signature 'XcmsExperiment'
rtime(object, adjusted = hasAdjustedRtime(object))

## S4 method for signature 'XcmsExperiment'
adjustedRtime(object)

## S4 method for signature 'XcmsExperiment'
hasFeatures(object, msLevel = integer())

## S4 replacement method for signature 'XcmsExperiment'
featureDefinitions(object) <- value

## S4 method for signature 'XcmsExperiment'
```

```
featureDefinitions(
  object,
  mz = numeric(),
  rt = numeric(),
  ppm = 0,
  type = c("any", "within", "apex_within"),
  msLevel = integer()
)

## S4 method for signature 'XcmsExperiment'
dropFeatureDefinitions(object, keepAdjustedRtime = FALSE)

## S4 method for signature 'XcmsExperiment'
filterFeatureDefinitions(object, features = integer())

## S4 method for signature 'XcmsExperiment'
hasFilledChromPeaks(object)

## S4 method for signature 'XcmsExperiment'
dropFilledChromPeaks(object)

## S4 method for signature 'XcmsExperiment'
quantify(object, ...)

## S4 method for signature 'XcmsExperiment'
featureValues(
  object,
  method = c("medret", "maxint", "sum"),
  value = "into",
  intensity = "into",
  filled = TRUE,
  missing = NA_real_,
  msLevel = integer()
)

## S4 method for signature 'XcmsExperiment'
chromatogram(
  object,
  rt = matrix(nrow = 0, ncol = 2),
  mz = matrix(nrow = 0, ncol = 2),
  aggregationFun = "sum",
  msLevel = 1L,
  chunkSize = 2L,
  isolationWindowTargetMz = NULL,
  return.type = c("XChromatograms", "MChromatograms"),
  include = character(),
  chromPeaks = c("apex_within", "any", "none"),
  BPPARAM = bpparam()
```

```
)

## S4 method for signature 'XcmsExperiment'
processHistory(object, type)

## S4 method for signature 'XcmsExperiment'
filterFile(
  object,
  file,
  keepAdjustedRtime = hasAdjustedRtime(object),
  keepFeatures = FALSE,
  ...
)

featureArea(
  object,
  mzmin = min,
  mzmax = max,
  rtmin = min,
  rtmax = max,
  features = character()
)

## S4 method for signature 'MsExperiment,missing'
plot(x, y, msLevel = 1L, peakCol = "#ff000060", ...)
```

Arguments

object	An XcmsExperiment object.
...	Additional optional parameters. For quantify: any parameter for the featureValues call used to extract the feature value matrix.
rt	For chromPeaks and featureDefinitions: numeric(2) defining the retention time range for which chromatographic peaks or features should be returned. The full range is used by default. For chromatogram: two column numerical matrix with each row representing the lower and upper retention time window(s) for the chromatograms. If not provided the full retention time range is used.
mz	For chromPeaks and featureDefinitions: numeric(2) optionally defining the m/z range for which chromatographic peaks or feature definitions should be returned. The full m/z range is used by default. For chromatogram: two-column numerical matrix with each row representing m/z range that should be aggregated into a chromatogram. If not provided the full m/z range of the data will be used (and hence a total ion chromatogram will be returned if aggregationFun = "sum" is used). For filterIsolationWindow: numeric(1) defining the m/z that should be contained within the spectra's isolation window.
msLevel.	For filterRt: ignored. filterRt will always filter by retention times on all MS levels regardless of this parameter. For chromatogram: integer with the MS level from which the chromatogram(s) should be extracted. Has to be either of length 1 or length equal to the numer of rows of the parameters mz and rt

defining the m/z and rt regions from which the chromatograms should be created. Defaults to `msLevel = 1L`. for `filterMsLevel`: `integer` defining the MS level(s) to which the data should be subset.

`file` For `filterFile`: `integer` with the indices of the samples (files) to which the data should be subsetted.

`aggregationFun` For `chromatogram`: `character(1)` defining the function that should be used to *aggregate* intensities for retention time (i.e. each spectrum) along the specified m/z range (parameter `mz`). Defaults to `aggregationFun = "sum"` and hence all intensities will be summed up. Alternatively, use `aggregationFun = "max"` to use the maximal intensity per m/z range to create a base peak chromatogram (BPC).

`msLevel` `integer` defining the MS level (or multiple MS level if the function supports it).

`isolationWindowTargetMz`
For `chromatogram`: `numeric` (of length equal to the number of rows of `rt` and `mz`) with the isolation window target m/z of the MS2 spectra from which the chromatgrom should be generated. For MS1 data (`msLevel = 1L`, the default), this parameter is ignored. See examples on `chromatogram` below for further information.

`chunkSize` For `chromatogram`: `integer(1)` defining the number of files from which the data should be loaded at a time into memory. Defaults to `chunkSize = 2L`.

`return.type` For `chromPeakData`: `character(1)` defining the class of the returned object. Can be either `"DataFrame"` (the default) or `"data.frame"`. For `chromatogram`: `character(1)` defining the type of the returned object. Currently only `return.type = "MChromatograms"` is supported.

`BPPARAM` For `chromatogram`: parallel processing setup. Defaults to `BPPARAM = bpparam()`. See `bpparam()` for more information.

`x` An `XcmsExperiment` object.

`i` For `[`: `integer` or `logical` defining the samples/files to subset.

`j` For `[`: not supported.

`drop` For `[`: ignored.

`keepAdjustedRtime`
`logical(1)`: whether adjusted retention times (if present) should be retained.

`value` For `featureValues`: `character(1)` defining which value should be reported for each feature in each sample. Can be any column of the `chromPeaks` matrix or `"index"` if simply the index of the assigned peak should be returned. Defaults to `value = "into"` thus the integrated peak area is reported.

`ppm` For `chromPeaks` and `featureDefinitions`: optional `numeric(1)` specifying the ppm by which the m/z range (defined by `mz` should be extended. For a value of `ppm = 10`, all peaks within `mz[1] - ppm / 1e6` and `mz[2] + ppm / 1e6` are returned.

`type` For `chromPeaks` and `featureDefinitions` and only if either `mz` and `rt` are defined too: `character(1)`: defining which peaks (or features) should be returned. For `type = "any"`: returns all chromatographic peaks or features also only partially overlapping any of the provided ranges. For `type = "within"`:

returns only peaks or features completely within the region defined by `mz` and/or `rt`. For `type = "apex_within"`: returns peaks or features for which the m/z and retention time of the peak's apex is within the region defined by `mz` and/or `rt`. For `processHistory`: restrict returned processing steps to specific types. Use `processHistoryTypes()` to list all supported values.

`isFilledColumn` For `chromPeaks`: `logical(1)` whether a column `"is_filled"` should be included in the returned `matrix` with the information whether a peak was detected or *only* filled-in. Note that this information is also provided in the `chromPeakData` data frame.

`keep` For `filterChromPeaks`: `logical`, `integer` or `character` specifying which chromatographic peaks to keep. If `logical` the length of `keep` needs to match the number of rows of `chromPeaks`. Alternatively, `keep` allows to specify the `index` (row) of peaks to keep or their ID (i.e. row name in `chromPeaks`).

`method` For `featureValues`: `character(1)` specifying the method to resolve multi-peak mappings within the same sample (correspondence analysis can assign more than one chromatographic peak within a sample to the same feature, e.g. if they are close in retention time). Options: `method = "medret"`: report the value for the chromatographic peak closest to the feature's median retention time. `method = "maxint"`: report the value for the chromatographic peak with the largest signal (parameter `intensity` allows to select the column in `chromPeaks` that should be used for *signal*). `method = "sum"`: sum the value for all chromatographic peaks in a sample assigned to the same feature. The default is `method = "medret"`. For `filterChromPeaks`: currently only `method = "keep"` is supported.

`adjusted` For `rtime,XcmsExperiment`: whether adjusted or *raw* retention times should be returned. The default is to return adjusted retention times, if available.

`features` For `filterFeatureDefinitions` and `featureArea`: `logical`, `integer` or `character` defining the features to keep or from which to extract the feature area, respectively. See function description for more information.

`intensity` For `featureValues`: `character(1)` specifying the name of the column in the `chromPeaks(objects)` matrix containing the intensity value of the peak that should be used for the conflict resolution if `method = "maxint"`.

`filled` For `featureValues`: `logical(1)` specifying whether values for filled-in peaks should be reported. For `filled = TRUE` (the default) filled peak values are returned, otherwise `NA` is reported for the respective features in the samples in which no peak was detected.

`missing` For `featureValues`: default value for missing values. Allows to define the value that should be reported for a missing peak intensity. Defaults to `missing = NA_real_`.

`include` For `chromatogram`: deprecated; use parameter `chromPeaks` instead.

`chromPeaks` For `chromatogram`: `character(1)` defining which chromatographic peaks should be returned. Can be either `chromPeaks = "apex_within"` (default) to return all chromatographic peaks with the m/z and RT of their apex within the m/z and retention time window, `chromPeaks = "any"` for all chromatographic peaks that are overlapping with the m/z - retention time window or `chromPeaks = "none"`

	to not include any chromatographic peaks. See also parameter type below for additional information.
keepFeatures	for most subsetting functions ([, filterFile): logical(1): wheter eventually present feature definitions should be retained in the returned (filtered) object.
mzmin	For featureArea: function to calculate the "mzmin" of a feature based on the "mzmin" values of the individual chromatographic peaks assigned to that feature. Defaults to mzmin = min.
mzmax	For featureArea: function to calculate the "mzmax" of a feature based on the "mzmax" values of the individual chromatographic peaks assigned to that feature. Defaults to mzmax = max.
rtmin	For featureArea: function to calculate the "rtmin" of a feature based on the "rtmin" values of the individual chromatographic peaks assigned to that feature. Defaults to rtmin = min.
rtmax	For featureArea: function to calculate the "rtmax" of a feature based on the "rtmax" values of the individual chromatographic peaks assigned to that feature. Defaults to rtmax = max.
y	For plot: should not be defined as it is not supported.
peakCol	For plot: defines the border color of the rectangles indicating the identified chromatographic peaks. Only a single color is supported. Defaults to 'peakCol = "#ff000060".

Subsetting and filtering

- [: subset an XcmsExperiment by **sample** (parameter i). Subsetting will by default drop correspondence results (as subsetting by samples will obviously affect the feature definition) and alignment results (adjusted retention times) while identified chromatographic peaks (for the selected samples) will be retained. Which preprocessing results should be kept or dropped can also be configured with optional parameters keepChromPeaks (by default TRUE), keepAdjustedRtime (by default FALSE) and keepFeatures (by default FALSE).
- filterChromPeaks: filter chromatographic peaks of an XcmsExperiment keeping only those specified with parameter keep. Returns the XcmsExperiment with the filtered data. Chromatographic peaks to retain can be specified either by providing their index in the chromPeaks matrix, their ID (rowname in chromPeaks) or with a logical vector with the same length than number of rows of chromPeaks. Assignment of chromatographic peaks are updated to eventually present feature definitions after filtering.
- filterFeatureDefinitions: filter feature definitions of an XcmsExperiment keeping only those defined with parameter features, which can be a logical of length equal to the number of features, an integer with the index of the features in featureDefinitions(object) to keep or a character with the feature IDs (i.e. row names in featureDefinitions(object)).
- filterFile: filter an XcmsExperiment (or MsExperiment) by *file* (sample). The index of the samples to which the data should be subsetted can be specified with parameter file. The sole purpose of this function is to provide backward compatibility with the MSnbase package. Wherever possible, the [function should be used instead for any sample-based subsetting. Parameters keepChromPeaks, keepAdjustedRtime and keepChromPeaks can be passed using .... Note also that in contrast to [, filterFile does not support subsetting in arbitrary order.

- `filterIsolationWindow`: filter the **spectra** within an `MsExperiment` or `XcmsExperiment` object keeping only those with an isolation window containing the specified m/z (i.e., keeping spectra with an `"isolationWindowLowerMz"` smaller than the user-provided `mz` and an `"isolationWindowUpperMz"` larger than `mz`). For an `XcmsExperiment` also all chromatographic peaks (and subsequently also features) are removed for which the range of their `"isolationWindowLowerMz"` and `"isolationWindowUpperMz"` (columns in `chromPeakData`) do not contain the user provided `mz`.
- `filterMsLevel`: filter the data of the `XcmsExperiment` or `MsExperiment` to keep only data of the MS level(s) specified with parameter `msLevel.`.
- `filterMz`, `filterMzRange`: filter the spectra within an `XcmsExperiment` or `MsExperiment` to the specified m/z range (parameter `mz`). For `XcmsExperiment` also identified chromatographic peaks and features are filtered keeping only those that are within the specified m/z range (i.e. for which the m/z of the peak apex is within the m/z range). Parameter `msLevels.` allows to restrict the filtering to only specified MS levels. By default data from all MS levels are filtered.
- `filterRt`: filter an `XcmsExperiment` keeping only data within the specified retention time range (parameter `rt`). This function will keep all preprocessing results present within the retention time range: all identified chromatographic peaks with the retention time of the apex position within the retention time range `rt` are retained along, if present, with the associated features. Parameter `msLevel.` is currently ignored, i.e. filtering will always performed on **all** MS levels of the object.

Functionality related to chromatographic peaks

- `chromatogram`: extract chromatographic data from a data set. Parameters `mz` and `rt` allow to define specific m/z - retention time regions to extract the data from (to e.g. for extracted ion chromatograms EICs). Both parameters are expected to be numerical two-column matrices with the first column defining the lower and the second the upper margin. Each row can define a separate m/z - retention time region. Currently the function returns a `MChromatograms()` object for `object` being a `MsExperiment` or, for `object` being an `XcmsExperiment`, either a `MChromatograms` or `XChromatograms()` depending on parameter `return.type` (can be either `"MChromatograms"` or `"XChromatograms"`). For the latter also chromatographic peaks detected within the provided m/z and retention times are returned. Parameter `chromPeaks` allows to specify which chromatographic peaks should be reported. See documentation on the `chromPeaks` parameter for more information. If the `XcmsExperiment` contains correspondence results, also the associated feature definitions will be included in the returned `XChromatograms`. By default the function returns chromatograms from MS1 data, but by setting parameter `msLevel = 2L` it is possible to e.g. extract also MS2 chromatograms. For `msLevel` other than 1 it is in addition important to also specify the `isolationWindowTargetMz` for which MS2 data should be extracted (e.g. for SWATH data MS2 spectra are created for different m/z isolation windows and the `isolationWindowTargetMz` parameter allows to define from which of these the MS2 chromatogram should be extracted. Note that in future more efficient data structures for chromatographic data will be available as well.
- `chromPeaks`: returns a `numeric` matrix with the identified chromatographic peaks. Each row represents a chromatographic peak identified in one sample (file). The number of columns depends on the peak detection algorithm (see `findChromPeaks()`) but most methods return the following columns: `"mz"` (intensity-weighted mean of the m/z values of all mass peaks included in the chromatographic peak), `"mzmin"` (smallest m/z value of any mass peak in the

chromatographic peak), "mzmax" (largest m/z value of any mass peak in the chromatographic peak), "rt" (retention time of the peak apex), "rtmin" (retention time of the first scan/mass peak of the chromatographic peak), "rtmax" (retention time of the last scan/mass peak of the chromatographic peak), "into" (integrated intensity of the chromatographic peak), "maxo" (maximal intensity of any mass peak of the chromatographic peak), "sample" (index of the sample in object in which the peak was identified). Parameters rt, mz, ppm, msLevel and type allow to extract subsets of identified chromatographic peaks from the object. See parameter description below for details.

- chromPeakData: returns a DataFrame with potential additional *annotations* for the identified chromatographic peaks. Each row in this DataFrame corresponds to a row (same index and row name) in the chromPeaks matrix. The default *annotations* are "ms_level" (the MS level in which the peak was identified) and "is_filled" (whether the chromatographic peak was *detected* (by findChromPeaks) or *filled-in* (by fillChromPeaks).
- chromPeakSpectra: extract MS spectra for identified chromatographic peaks. This can be either all (full scan) MS1 spectra with retention times between the retention time range of a chromatographic peak, all MS2 spectra (if present) with a retention time within the retention time range of a (MS1) chromatographic peak and a precursor m/z within the m/z range of the chromatographic peak or single, selected spectra depending on their total signal or highest signal. Parameter msLevel allows to define from which MS level spectra should be extracted, parameter method allows to define if all or selected spectra should be returned. See chromPeakSpectra() for details.
- dropChromPeaks: removes (all) chromatographic peak detection results from object. This will also remove any correspondence results (i.e. features) and eventually present adjusted retention times from the object if the alignment was performed **after** the peak detection. Alignment results (adjusted retention times) can be retained if parameter keepAdjustedRtime is set to TRUE.
- dropFilledChromPeaks: removes chromatographic peaks added by gap filling with fillChromPeaks.
- fillChromPeaks: perform *gap filling* to integrate signal missing values in samples in which no chromatographic peak was found. This depends on correspondence results, hence groupChromPeaks needs to be called first. For details and options see fillChromPeaks().
- findChromPeaks: perform chromatographic peak detection. See findChromPeaks() for details.
- hasChromPeaks: whether the object contains peak detection results. Parameter msLevel allows to check whether peak detection results are available for the specified MS level(s).
- hasFilledChromPeaks: whether gap-filling results (i.e., filled-in chromatographic peaks) are present.
- manualChromPeaks: *manually* add chromatographic peaks by defining their m/z and retention time ranges. See manualChromPeaks() for details and examples.
- plotChromPeakImage: show the *density* of identified chromatographic peaks per file along the retention time. See plotChromPeakImage() for details.
- plotChromPeaks: indicate identified chromatographic peaks from one sample in the RT-m/z space. See plotChromPeaks() for details.
- refineChromPeaks: *refines* identified chromatographic peaks in object. See refineChromPeaks() for details.

Functionality related to alignment

- `adjustedRtime`: extract adjusted retention times. This is just an alias for `rtime(object, adjusted = TRUE)`.
- `adjustRtime`: performs retention time adjustment (alignment) of the data. See `adjustRtime()` for details.
- `applyAdjustedRtime`: replaces the original (raw) retention times with the adjusted ones. See `applyAdjustedRtime()` for more information.
- `dropAdjustedRtime`: drops alignment results (adjusted retention time) from the result object. This also reverts the retention times of identified chromatographic peaks if present in the result object. Note that any results from a correspondence analysis (i.e. feature definitions) will be dropped too (if the correspondence analysis was performed **after** the alignment). This can be overruled with `keepAdjustedRtime = TRUE`.
- `hasAdjustedRtime`: whether alignment was performed on the object (i.e., the object contains alignment results).
- `plotAdjustedRtime`: plot the alignment results; see `plotAdjustedRtime()` for more information.

Functionality related to correspondence analysis

- `dropFeatureDefinitions`: removes any correspondence analysis results from `object` as well as any filled-in chromatographic peaks. By default (with parameter `keepAdjustedRtime = FALSE`) also all alignment results will be removed if alignment was performed **after** the correspondence analysis. This can be overruled with `keepAdjustedRtime = TRUE`.
- `featureArea`: returns a `matrix` with columns `"mzmin"`, `"mzmax"`, `"rtmin"` and `"rtmax"` with the m/z and retention time range for each feature (row) in `object`. By default these represent the minimal m/z and retention times as well as maximal m/z and retention times for all chromatographic peaks assigned to that feature. Parameter `features` allows to extract these values for selected features only. Parameters `mzmin`, `mzmax`, `rtmin` and `rtmax` allow to define the function to calculate the reported `"mzmin"`, `"mzmax"`, `"rtmin"` and `"rtmax"` values.
- `featureChromatograms`: extract ion chromatograms (EICs) for each feature in `object`. See `featureChromatograms()` for more details.
- `featureDefinitions`: returns a `data.frame` with feature definitions or an empty `data.frame` if no correspondence analysis results are present. Parameters `msLevel`, `mz`, `ppm` and `rt` allow to define subsets of feature definitions that should be returned with the parameter `type` defining how these parameters should be used to subset the returned `data.frame`. See parameter descriptions for details.
- `featureSpectra`: returns a `Spectra()` or `List` of `Spectra` with (MS1 or MS2) spectra associated to each feature. See `featureSpectra()` for more details and available parameters.
- `featuresSummary`: calculate a simple summary on features. See `featureSummary()` for details.
- `groupChromPeaks`: performs the correspondence analysis (i.e., grouping of chromatographic peaks into LC-MS *features*). See `groupChromPeaks()` for details.
- `hasFeatures`: whether correspondence analysis results are presentin in `object`. The optional parameter `msLevel` allows to define the MS level(s) for which it should be determined if feature definitions are available.

- `overlappingFeatures`: identify features that overlapping or close in m/z - rt dimension. See `overlappingFeatures()` for more information.

Extracting data and results from an `XcmsExperiment`

Preprocessing results can be extracted using the following functions:

- `chromPeaks`: extract identified chromatographic peaks. See section on chromatographic peak detection for details.
- `featureDefinitions`: extract the definition of *features* (chromatographic peaks grouped across samples). See section on correspondence analysis for details.
- `featureValues`: extract a `matrix` of *values* for features from each sample (file). Rows are features, columns samples. Which *value* should be returned can be defined with parameter `value`, which can be any column of the `chromPeaks` matrix. By default (`value = "into"`) the integrated chromatographic peak intensities are returned. With parameter `msLevel` it is possible to extract values for features from certain MS levels. During correspondence analysis, more than one chromatographic peak per sample can be assigned to the same feature (e.g. if they are very close in retention time). Parameter `method` allows to define the strategy to deal with such cases: `method = "medret"`: report the value from the chromatographic peak with the apex position closest to the feautre's median retention time. `method = "maxint"`: report the value from the chromatographic peak with the largest signal (parameter `intensity` allows to define the column in `chromPeaks` that should be selected; defaults to `intensity = "into"`). method = "sum"‘: sum the values for all chromatographic peaks assigned to the feature in the same sample.
- `quantify`: extract the correspondence analysis results as a `SummarizedExperiment()`. The feature *values* are used as `assay` in the returned `SummarizedExperiment`, `rowData` contains the `featureDefinitions` (without column `"peakidx"`) and `colData` the `sampleData` of `object`. Additional parameters to the `featureValues` function (that is used to extract the feature value matrix) can be passed *via* ....

Visualization

- `plot`: plot for each file the position of individual peaks in the m/z - retention time space (with color-coded intensity) and a base peak chromatogram. This function should ideally be called only on a data subset (i.e. after using `filterRt` and `filterMz` to restrict to a region of interest). Parameter `msLevel` allows to define from which MS level the plot should be created. If `x` is a `XcmsExperiment` with available identified chromatographic peaks, also the region defining the peaks are indicated with a rectangle. Parameter `peakCol` allows to define the color of the border for these rectangles.
- `plotAdjustedRtime`: plot the alignment results; see `plotAdjustedRtime()` for more information.
- `plotChromPeakImage`: show the *density* of identified chromatographic peaks per file along the retention time. See `plotChromPeakImage()` for details.
- `plotChromPeaks`: indicate identified chromatographic peaks from one sample in the RT-m/z space. See `plotChromPeaks()` for details.

General functionality and functions for backward compatibility

- `uniqueMsLevels`: returns the unique MS levels of the spectra in `object`.

The functions listed below ensure compatibility with the *older* `XCMSnExp()` xcms result object.

- `fileNames`: returns the original data file names for the spectra data. Ideally, the `dataOrigin` or `dataStorage` spectra variables from the object's `spectra` should be used instead.
- `fromFile`: returns the file (sample) index for each spectrum within `object`. Generally, subsetting by sample using the `[` is the preferred way to get spectra from a specific sample.
- `polarity`: returns the polarity information for each spectrum in `object`.
- `processHistory`: returns a `list` with ProcessHistory *process history* objects that contain also the parameter object used for the different processings. Optional parameter `type` allows to query for specific processing steps.
- `rtime`: extract retention times of the **spectra** from the `MsExperiment` or `XcmsExperiment` object. It is thus a shortcut for `rtime(spectra(object))` which would be the preferred way to extract retention times from an `MsExperiment`. The `rtime` method for `XcmsExperiment` has an additional parameter `adjusted` which allows to define whether adjusted retention times (if present - `adjusted = TRUE`) or *raw* retention times (`adjusted = FALSE`) should be returned. By default adjusted retention times are returned if available.

Differences compared to the `XCMSnExp()` object

- Subsetting by `[` supports arbitrary ordering.

Author(s)

Johannes Rainer

Examples

```
## Creating a MsExperiment object representing the data from an LC-MS
## experiment.
library(MsExperiment)

## Defining the raw data files
fls <- 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"))

## Defining a data frame with the sample characterization
df <- data.frame(mzML_file = basename(fls),
                 sample = c("ko15", "ko16", "ko18"))
## Importing the data. This will initialize a `Spectra` object representing
## the raw data and assign these to the individual samples.
mse <- readMsExperiment(spectraFiles = fls, sampleData = df)

## Extract a total ion chromatogram and base peak chromatogram
## from the data
bpc <- chromatogram(mse, aggregationFun = "max")
tic <- chromatogram(mse)
```

```
## Plot them
par(mfrow = c(2, 1))
plot(bpc, main = "BPC")
plot(tic, main = "TIC")

## Extracting MS2 chromatographic data
##
## To show how MS2 chromatograms can be extracted we first load a DIA
## (SWATH) data set.
mse_dia <- readMsExperiment(system.file("TripleTOF-SWATH",
    "PestMix1_SWATH.mzML", package = "msdata"))

## Extracting MS2 chromatogram requires also to specify the isolation
## window from which to extract the data. Without that chromatograms
## will be empty:
chr_ms2 <- chromatogram(mse_dia, msLevel = 2L)
intensity(chr_ms2[[1L]])

## First we list available isolation windows
table(isolationWindowTargetMz(spectra(mse_dia)))

## We can then extract the TIC of MS2 data for a specific isolation window
chr_ms2 <- chromatogram(mse_dia, msLevel = 2L,
    isolationWindowTargetMz = 244.05)
plot(chr_ms2)

####
## Chromatographic peak detection

## Perform peak detection on the data using the centWave algorith. Note
## that the parameters are chosen to reduce the run time of the example.
p <- CentWaveParam(noise = 10000, snthresh = 40, prefilter = c(3, 10000))
xmse <- findChromPeaks(mse, param = p)
xmse

## Have a quick look at the identified chromatographic peaks
head(chromPeaks(xmse))

## Extract chromatographic peaks identified between 3000 and 3300 seconds
chromPeaks(xmse, rt = c(3000, 3300), type = "within")

## Extract ion chromatograms (EIC) for the first two chromatographic
## peaks.
chrs <- chromatogram(xmse,
    mz = chromPeaks(xmse)[1:2, c("mzmin", "mzmax")],
    rt = chromPeaks(xmse)[1:2, c("rtmin", "rtmax")])

## An EIC for each sample and each of the two regions was extracted.
## Identified chromatographic peaks in the defined regions are extracted
## as well.
chrs
```

```
## Plot the EICs for the second defined region
plot(chrs[2, ])

## Subsetting the data to the results (and data) for the second sample
a <- xmse[2]
nrow(chromPeaks(xmse))
nrow(chromPeaks(a))

## Filtering the result by retention time: keeping all spectra and
## chromatographic peaks within 3000 and 3500 seconds.
xmse_sub <- filterRt(xmse, rt = c(3000, 3500))
xmse_sub
nrow(chromPeaks(xmse_sub))

## Perform an initial feature grouping to allow alignment using the
## peak groups method:
pdp <- PeakDensityParam(sampleGroups = rep(1, 3))
xmse <- groupChromPeaks(xmse, param = pdp)

## Perform alignment using the peak groups method.
pgp <- PeakGroupsParam(span = 0.4)
xmse <- adjustRtime(xmse, param = pgp)

## Visualizing the alignment results
plotAdjustedRtime(xmse)

## Performing the final correspondence analysis
xmse <- groupChromPeaks(xmse, param = pdp)

## Show the definition of the first 6 features
featureDefinitions(xmse) |> head()

## Extract the feature values; show the results for the first 6 rows.
featureValues(xmse) |> head()

## The full results can also be extracted as a `SummarizedExperiment`
## that would eventually simplify subsequent analyses with other packages.
## Any additional parameters passed to the function are passed to the
## `featureValues` function that is called to generate the feature value
## matrix.
se <- quantify(xmse, method = "sum")

## EICs for all features can be extracted with the `featureChromatograms`
## function. Note that, depending on the data set, extracting this for
## all features might take some time. Below we extract EICs for the
## first 10 features by providing the feature IDs.
chrs <- featureChromatograms(xmse,
    features = rownames(featureDefinitions(xmse))[1:10])
chrs

plot(chrs[3, ])
```

filterFeatures *Filtering of features based on conventional quality assessment*

Description

When dealing with metabolomics results, it is often necessary to filter features based on certain criteria. These criteria are typically derived from statistical formulas applied to full rows of data, where each row represents a feature and its abundance of signal in each samples. The `filterFeatures` function filters features based on these conventional quality assessment criteria. Multiple types of filtering are implemented and can be defined by the `filter` argument.

Supported `filter` arguments are:

- `RsdFilter`: Calculates the relative standard deviation (i.e. coefficient of variation) in abundance for each feature in QC (Quality Control) samples and filters them in the input object according to a provided threshold.
- `DratioFilter`: Computes the D-ratio or *dispersion ratio*, defined as the standard deviation in abundance for QC samples divided by the standard deviation for biological test samples, for each feature and filters them according to a provided threshold.
- `PercentMissingFilter`: Determines the percentage of missing values for each feature in the various sample groups and filters them according to a provided threshold.
- `BlankFlag`: Identifies features where the mean abundance in test samples is lower than a specified multiple of the mean abundance of blank samples. This can be used to flag features that result from contamination in the solvent of the samples. A new column `possible_contaminants` is added to the `featureDefinitions` (`XcmsExperiment` object) or `rowData` (`SummarizedExperiment` object) reflecting this.

For specific examples, see the help pages of the individual parameter classes listed above.

Arguments

`object`	`XcmsExperiment` or `SummarizedExperiment`. For an `XcmsExperiment` object, the `featureValues(object)` will be evaluated, and for `Summarizedesxperiment` the `assay(object, assay)`. The object will be filtered.
`filter`	The parameter object selecting and configuring the type of filtering. It can be one of the following classes: `RsdFilter`, `DratioFilter`, `PercentMissingFilter` or `BlankFlag`.
`assay`	For filtering of `SummarizedExperiment` objects only. Indicates which assay the filtering will be based on. Note that the features for the entire object will be removed, but the computations are performed on a single assay. Default is 1, which means the first assay of the `object` will be evaluated.
`...`	Optional parameters. For `object` being an `XcmsExperiment`: parameters for the `featureValues()` call.

Author(s)

Philippine Louail

References

Broadhurst D, Goodacre R, Reinke SN, Kuligowski J, Wilson ID, Lewis MR, Dunn WB. Guidelines and considerations for the use of system suitability and quality control samples in mass spectrometry assays applied in untargeted clinical metabolomic studies. Metabolomics. 2018;14(6):72. doi: 10.1007/s11306-018-1367-3. Epub 2018 May 18. PMID: 29805336; PMCID: PMC5960010.

Examples

```
## See the vignettes for more detailed examples
library(MsExperiment)

## Load a test data set with features defined.
test_xcms <- loadXcmsData()
## Set up parameter to filter based on coefficient of variation. By setting
## the filter such as below, features that have a coefficient of variation
## superior to 0.3 in QC samples will be removed from the object `test_xcms`
## when calling the `filterFeatures` function.

rsd_filter <- RsdFilter(threshold = 0.3,
                        qcIndex = sampleData(test_xcms)$sample_type == "QC")

filtered_data_rsd <- filterFeatures(object = test_xcms, filter = rsd_filter)

## Set up parameter to filter based on D-ratio. By setting the filter such
## as below, features that have a D-ratio computed based on their abundance
## between QC and study samples superior to 0.5 will be removed from the
## object `test_xcms`.

dratio_filter <- DratioFilter(threshold = 0.5,
                 qcIndex = sampleData(test_xcms)$sample_type == "QC",
                 studyIndex = sampleData(test_xcms)$sample_type == "study")

filtered_data_dratio <- filterFeatures(object = test_xcms,
                                       filter = dratio_filter)

## Set up parameter to filter based on the percent of missing data.
## Parameter f should represent the sample group of samples, for which the
## percentage of missing values will be evaluated. As the setting is defined
## bellow, if a feature as less (or equal) to 30% missing values in one
## sample group, it will be kept in the `test_xcms` object.

missing_data_filter <- PercentMissingFilter(threshold = 30,
                                       f = sampleData(test_xcms)$sample_type)

filtered_data_missing <- filterFeatures(object = test_xcms,
                                        filter = missing_data_filter)

## Set up parameter to flag possible contaminants based on blank samples'
## abundance. By setting the filter such as below, features that have mean
## abundance ratio between blank(here use study as an example) and QC
## samples less than 2 will be marked as `TRUE` in an extra column named
## `possible_contaminants` in the `featureDefinitions` table of the object
```

```
## `test_xcms`.

filter <- BlankFlag(threshold = 2,
                    qcIndex = sampleData(test_xcms)$sample_type == "QC",
                    blankIndex = sampleData(test_xcms)$sample_type == "study")
filtered_xmse <- filterFeatures(test_xcms, filter)
```

`filtfft` *Apply an convolution filter using an FFT*

Description

Expands a vector to the length of the filter and then convolutes it using two successive FFTs.

Usage

```
filtfft(y, filt)
```

Arguments

`y`	numeric vector of data to be filtered
`filt`	filter with length `nextn(length(y))`

Value

A numeric vector the same length as y.

Author(s)

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`findChromPeaks` *Chromatographic Peak Detection*

Description

The `findChromPeaks` method performs chromatographic peak detection on LC/GC-MS data. The peak detection algorithm can be selected, and configured, using the `param` argument.

Supported `param` objects are:

- `CentWaveParam()`: chromatographic peak detection using the *centWave* algorithm.
- `CentWavePredIsoParam()`: *centWave* with predicted isotopes. Peak detection uses a two-step centWave-based approach considering also feature isotopes.
- `MatchedFilterParam()`: peak detection using the *matched filter* algorithm.
- `MassifquantParam()`: peak detection using the Kalman filter-based *massifquant* method.
- `MSWParam()`: single-spectrum non-chromatography MS data peak detection.

For specific examples see the help pages of the individual parameter classes listed above.

Usage

```
findChromPeaks(object, param, ...)

## S4 method for signature 'MsExperiment,Param'
findChromPeaks(
  object,
  param,
  msLevel = 1L,
  chunkSize = 2L,
  ...,
  BPPARAM = bpparam()
)

## S4 method for signature 'XcmsExperiment,Param'
findChromPeaks(
  object,
  param,
  msLevel = 1L,
  chunkSize = 2L,
  add = FALSE,
  ...,
  BPPARAM = bpparam()
)
```

Arguments

object	The data object on which to perform the peak detection. Can be an OnDiskMSnExp(), XCMSnExp(), MChromatograms() or MsExperiment() object.
param	The parameter object selecting and configuring the algorithm.
...	Optional parameters.
msLevel	integer(1) defining the MS level on which the chromatographic peak detection should be performed.
chunkSize	integer(1) for object being an MsExperiment or XcmsExperiment(): defines the number of files (samples) for which the full peaks data (m/z and intensity values) should be loaded into memory at the same time. Peak detection is then performed in parallel (per sample) on this subset of loaded data. This setting thus allows to balance between memory demand and speed (due to parallel processing) of the peak detection. Because parallel processing can only performed on the subset of data loaded currently into memory (in each iteration), the value for chunkSize should be match the defined parallel setting setup. Using a parallel processing setup using 4 CPUs (separate processes) but using chunkSize = 1will not perform any parallel processing, as only the data from one sample i =-1the peak detection will be performed separately, and in parallel, for each sample. Th *backends* (see eventually Spectra() for details).
BPPARAM	Parallel processing setup. Uses by default the system-wide default setup. See bpparam() for more details.

add — logical(1) (if object contains already chromatographic peaks, i.e. is either an XCMSnExp or XcmsExperiment) whether chromatographic peak detection results should be **added** to existing results. By default (add = FALSE) any additional findChromPeaks call on a result object will remove previous results.

Author(s)

Johannes Rainer

See Also

plotChromPeaks() to plot identified chromatographic peaks for one file.

refineChromPeaks() for methods to *refine* or clean identified chromatographic peaks.

manualChromPeaks() to manually add/define chromatographic peaks.

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

---

findChromPeaks,Chromatogram,CentWaveParam-method

centWave-based peak detection in purely chromatographic data

Description

findChromPeaks on a Chromatogram or MChromatograms 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.

After chromatographic peak detection, identified peaks can also be *refined* with the refineChromPeaks() method, which can help to reduce peak detection artifacts.

Usage

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

## S4 method for signature 'MChromatograms,CentWaveParam'
findChromPeaks(object, param, BPPARAM = bpparam(), ...)

## S4 method for signature 'MChromatograms,MatchedFilterParam'
findChromPeaks(object, param, BPPARAM = BPPARAM, ...)
```

Arguments

object	a Chromatogram or MChromatograms 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.
BPPARAM	a parameter class specifying if and how parallel processing should be performed (only for XChromatograms objects). It defaults to bpparam(). See bpparam() for more information.

Value

If called on a Chromatogram object, the method returns an XChromatogram object with the identified peaks. See peaksWithCentWave() for details on the peak matrix content.

Author(s)

Johannes Rainer

See Also

peaksWithCentWave() for the downstream function and centWave for details on the method.

Examples

```
library(MSnbase)
## Loading a test data set with identified chromatographic peaks
faahko_sub <- loadXcmsData("faahko_sub2")
faahko_sub <- filterRt(faahko_sub, c(2500, 3700))

##
od <- as(filterFile(faahko_sub, 1L), "MsExperiment")

## 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
xchr <- findChromPeaks(chr, CentWaveParam())
xchr

## Plot data and identified peaks.
plot(xchr)

library(MsExperiment)
library(xcms)
## Perform peak detection on an MChromatograms object

fls <- 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"))
```

```
od3 <- readMsExperiment(fls)

## Disable parallel processing for this example
register(SerialParam())

## Extract chromatograms for a m/z - retention time slice
chrs <- chromatogram(od3, mz = 344, rt = c(2500, 3500))

## Perform peak detection using CentWave
xchrs <- findChromPeaks(chrs, param = CentWaveParam())
xchrs

## Extract the identified chromatographic peaks
chromPeaks(xchrs)

## plot the result
plot(xchrs)
```

`findChromPeaks,Chromatogram,MatchedFilterParam-method`
matchedFilter-based peak detection in purely chromatographic data

---

Description

`findChromPeaks` on a Chromatogram or MChromatograms 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 MChromatograms 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

```
## Loading a test data set with identified chromatographic peaks
faahko_sub <- loadXcmsData("faahko_sub2")
faahko_sub <- filterRt(faahko_sub, c(2500, 3700))

##
od <- as(filterFile(faahko_sub, 1L), "MsExperiment")

## 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
xchr <- findChromPeaks(chr, MatchedFilterParam())

## Plot the identified peaks
plot(xchr)
```

---

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Usage

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

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

## 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

## S4 method for signature 'CentWaveParam'
as.list(x, ...)
```

Arguments

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

mzdiff numeric(1) representing the minimum difference in m/z dimension 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. In detail, a first rough estimate of the noise is calculated and peak detection is performed only in regions in which multiple sequential signals are higher than this first estimated baseline/noise level.

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.

extendLengthMSW

Option to force centWave to use all scales when running centWave rather than truncating with the EIC length. Uses the "open" method to extend the EIC to a integer base-2 length prior to being passed to convolve rather than the default "reflect" method. See https://github.com/sneumann/xcms/issues/445 for more information.

verboseBetaColumns

Option to calculate two additional metrics of peak quality via comparison to an idealized bell curve. Adds beta_cor and beta_snr to the chromPeaks output, corresponding to a Pearson correlation coefficient to a bell curve with several degrees of skew as well as an estimate of signal-to-noise using the residuals from the best-fitting bell curve. See https://github.com/sneumann/xcms/pull/685 and https://doi.org/10.1186/s12859-023-05533-4 for more information.

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.
...	ignored.
value	The value for the slot.
f	For integrate: a CentWaveParam object.
x	The parameter 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

ppm,peakwidth,snthresh,prefilter,mzCenterFun,integrate,mzdiff,fitgauss,noise,verboseColumns,roiList
: See corresponding parameter above. 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 OnDiskMSnExp objects (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 Böttcher, 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: findChromPeaks(), 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, prefilter = c(3, 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 `readMsExperiment` function
## from the MsExperiment package
library(faahKO)
library(xcms)
library(MsExperiment)
fls <- dir(system.file("cdf/KO", package = "faahKO"), recursive = TRUE,
           full.names = TRUE)
raw_data <- readMsExperiment(fls[1])

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

---

findChromPeaks-centWaveWithPredIsoROIs

Two-step centWave peak detection considering also isotopes

Description

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

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

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

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

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

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

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

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

Usage

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

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

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

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

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

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

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

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

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

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

Arguments

ppm	numeric(1) defining the maximal tolerated m/z deviation in consecutive scans in parts per million (ppm) for the initial ROI definition.
peakwidth	numeric(2) with the expected approximate peak width in chromatographic space. Given as a range (min, max) in seconds.
snthresh	numeric(1) defining the signal to noise ratio cutoff.

prefilter numeric(2): c(k, I) specifying the prefilter step for the first analysis step (ROI detection). Mass traces are only retained if they contain at least k peaks with intensity >= I.

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

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

mzdiff numeric(1) representing the minimum difference in m/z dimension 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. In detail, a first rough estimate of the noise is calculated and peak detection is performed only in regions in which multiple sequential signals are higher than this first estimated baseline/noise level.

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.

extendLengthMSW
Option to force centWave to use all scales when running centWave rather than truncating with the EIC length. Uses the "open" method to extend the EIC to a integer base-2 length prior to being passed to convolve rather than the default "reflect" method. See https://github.com/sneumann/xcms/issues/445 for more information.

verboseBetaColumns
Option to calculate two additional metrics of peak quality via comparison to an idealized bell curve. Adds beta_cor and beta_snr to the chromPeaks output,

corresponding to a Pearson correlation coefficient to a bell curve with several degrees of skew as well as an estimate of signal-to-noise using the residuals from the best-fitting bell curve. See https://github.com/sneumann/xcms/pull/685 and https://doi.org/10.1186/s12859-023-05533-4 for more information.

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

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

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

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

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

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

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

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

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

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

`...`
: ignored.

`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

ppm,peakwidth,snthresh,prefilter,mzCenterFun,integrate,mzdiff,fitgauss,noise,verboseColumns,roiList
See corresponding parameter 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 OnDiskMSnExp objects (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: findChromPeaks(), 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'
ppm(object)

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

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

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

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

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

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

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

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

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

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

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

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

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

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

```
fitgauss(object)

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Arguments

ppm	numeric(1) defining the maximal tolerated m/z deviation in consecutive scans in parts per million (ppm) for the initial ROI definition.
peakwidth	numeric(2). Only the first element is used by massifquant, which specifices the minimum peak length in time scans. For withWave = TRUE the second argument represents the maximum peak length subject to being greater than the mininum peak length (see also documentation of do_findChromPeaks_centWave).
snthresh	numeric(1) defining the signal to noise ratio cutoff.
prefilter	numeric(2). The first argument is only used if (withWave = TRUE); see findChromPeaks-centWave for details. The second argument specifies the 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 prediciton margin of error. A real centroid belonging to a bonafide peak must fall within the KF prediction margin of error. Much like in the construction of a confidence interval, criticalVal loosely translates to be a multiplier of the standard error of the prediction reported by the Kalman Filter. If the peak in the XC-MS sample have a small mass deviance in ppm error, a smaller critical value might be better and vice versa.
consecMissedLimit	integer(1) Suggested values: (1,2,3). While a peak is in the proces of being detected by a Kalman Filter, the Kalman Filter may not find a predicted centroid in every scan. After 1 or more consecutive failed predictions, this setting informs Massifquant when to stop a Kalman Filter from following a candidate peak.

unions	integer(1) set to 1 if apply t-test union on segmentation; set to 0 if no t-test to be applied on chromatographically continous peaks sharing same m/z range. Explanation: With very few data points, sometimes a Kalman Filter stops tracking a peak prematurely. Another Kalman Filter is instantiated and begins following the rest of the signal. Because tracking is done backwards to forwards, this algorithmic defect leaves a real peak divided into two segments or more. With this option turned on, the program identifies segmented peaks and combines them (merges them) into one with a two sample t-test. The potential danger of this option is that some truly distinct peaks may be merged.
checkBack	integer(1) set to 1 if turned on; set to 0 if turned off. The convergence of a Kalman Filter to a peak's precise m/z mapping is very fast, but sometimes it incorporates erroneous centroids as part of a peak (especially early on). The scanBack option is an attempt to remove the occasional outlier that lies beyond the converged bounds of the Kalman Filter. The option does not directly affect identification of a peak because it is a postprocessing measure; it has not shown to be a extremely useful thus far and the default is set to being turned off.
withWave	logical(1) if TRUE, the peaks identified first with Massifquant are subsequently filtered with the second step of the centWave algorithm, which includes wavelet estimation.
object	For findChromPeaks: an OnDiskMSnExp object containing the MS- and all other experiment-relevant data. For all other methods: a parameter object.
param	An MassifquantParam object containing all settings for the massifquant algorithm.
BPPARAM	A parameter class specifying if and how parallel processing should be performed. It defaults to bpparam. See documentation of the BiocParallel for more details. If parallel processing is enabled, peak detection is performed in parallel on several of the input samples.
return.type	Character specifying what type of object the method should return. Can be either "XCMSnExp" (default), "list" or "xcmsSet".
msLevel	integer(1) defining the MS level on which the peak detection should be performed. Defaults to msLevel = 1.
...	ignored.
value	The value for the slot.
f	For integrate: a MassifquantParam object.

Details

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

visual inspection of peak identification is the best suggested tool for quick optimization. The ppm and checkBack parameters have shown less influence than the other parameters and exist to give users flexibility and better accuracy.

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

Value

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

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

Slots

ppm,peakwidth,snthresh,prefilter,mzCenterFun,integrate,mzdiff,fitgauss,noise,verboseColumns,critica
: See corresponding parameter above. 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 OnDiskMSnExp objects (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: findChromPeaks(), findChromPeaks-centWave, findChromPeaks-centWaveWithPredIso
findChromPeaks-matchedFilter, findPeaks-MSW

Examples

```
## Create a MassifquantParam object.
mqp <- MassifquantParam()
## Change snthresh prefilter parameters
snthresh(mqp) <- 30
prefilter(mqp) <- c(6, 10000)
mqp

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

`findChromPeaks-matchedFilter`

Peak detection in the chromatographic time domain

Description

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Usage

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

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

## S4 method for signature 'MatchedFilterParam'
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.
...	ignored.
value	The value for the slot.
x	For max: a MatchedFilterParam object.

Details

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

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

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

Value

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

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

Slots

binSize,impute,baseValue,distance,fwhm,sigma,max,snthresh,steps,mzdiff,index See corresponding parameter above. 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 OnDiskMSnExp objects (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: findChromPeaks(), findChromPeaks-centWave, findChromPeaks-centWaveWithPredIso
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], 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"
res <- findChromPeaks(raw_data, param = mfp)
head(chromPeaks(res))
```

---

findChromPeaksIsolationWindow

Data independent acquisition (DIA): peak detection in isolation windows

---

Description

The findChromPeaksIsolationWindow function allows to perform a chromatographic peak detection in MS level > 1 spectra of certain isolation windows (e.g. SWATH pockets). The function performs a peak detection, separately for all spectra belonging to the same isolation window and adds them to the chromPeaks() matrix of the result object. Information about the isolation window in which they were detected is added to chromPeakData() data frame.

Note that peak detection with this method does not remove previously identified chromatographic peaks (e.g. on MS1 level using the findChromPeaks() function but adds newly identified peaks to the existing chromPeaks() matrix.

Isolation windows can be defined with the `isolationWindow` parameter, that by default uses the definition of `isolationWindowTargetMz()`, i.e. chromatographic peak detection is performed for all spectra with the same isolation window target m/z (seprarately for each file). The parameter `param` allows to define and configure the peak detection algorithm (see `findChromPeaks()` for more information).

Usage

```
findChromPeaksIsolationWindow(object, ...)

## S4 method for signature 'MsExperiment'
findChromPeaksIsolationWindow(
  object,
  param,
  msLevel = 2L,
  isolationWindow = isolationWindowTargetMz(spectra(object)),
  chunkSize = 2L,
  ...,
  BPPARAM = bpparam()
)

## S4 method for signature 'OnDiskMSnExp'
findChromPeaksIsolationWindow(
  object,
  param,
  msLevel = 2L,
  isolationWindow = isolationWindowTargetMz(object),
  ...
)
```

Arguments

`object`	`MsExperiment`, `XcmsExperiment`, `OnDiskMSnExp` or `XCMSnExp` object with the DIA data.
`...`	currently not used.
`param`	Peak detection parameter object, such as a CentWaveParam object defining and configuring the chromographic peak detection algorithm. See also `findChromPeaks()` for more details.
`msLevel`	`integer(1)` specifying the MS level in which the peak detection should be performed. By default `msLevel = 2L`.
`isolationWindow`	`factor` or similar defining the isolation windows in which the peak detection should be performed with length equal to the number of spectra in `object`.
`chunkSize`	if `object` is an `MsExperiment` or `XcmsExperiment`: `integer(1)` defining the number of files (samples) that should be loaded into memory and processed at a time. See `findChromPeaks()` for more information.
`BPPARAM`	if `object` is an `MsExperiment` or `XcmsExperiment`: parallel processing setup. See `bpparam()` for more information.

Value

An XcmsExperiment or XCMSnExp object with the chromatographic peaks identified in spectra of each isolation window from each file added to the chromPeaks matrix. Isolation window definition for each identified peak are stored as additional columns in chromPeakData().

Author(s)

Johannes Rainer, Michael Witting

See Also

reconstructChromPeakSpectra() for the function to reconstruct MS2 spectra for each MS1 chromatographic peak.

---

findEqualGreater *Find values in sorted vectors*

Description

Find values in sorted vectors.

Usage

```
findEqualGreater(x, value)
findEqualLess(x, value)
findEqualGreaterM(x, values)
findRange(x, values, NAOK = FALSE)
```

Arguments

x	numeric vector sorted in increasing order
value	value to find in x
values	numeric values to find in x
NAOK	don't check for NA values in x

Details

findEqualGreater finds the index of the first value in x that is equal or greater than value. findEqualLess does same except that it finds equal or less. findEqualGreaterM creates an index of a vector by finding specified values. findRange locates the start and stop indicides of a range of two x values.

The only things that save time at this point are findeEqualGreaterM (when the length of values approaches the lenght of x) and findRange (when NAOK is set to TRUE). They run in log(N) and N time, respectively.

Value

An integer vector with the position(s) of the values(s).

Author(s)

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

`findMZ` *Find fragment ions in xcmsFragment objects*

Description

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

Usage

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

Arguments

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

Details

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

Value

A data frame with the following columns:

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

Author(s)

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

References

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

See Also

findneutral,

Examples

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

## End(Not run)
```

---

findneutral *Find neutral losses in xcmsFragment objects*

Description

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

Usage

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

Arguments

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

Details

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

Value

A data frame with the following columns:

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

Author(s)

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

References

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

See Also

findMZ,

Examples

```
## Not run:
    library(msdata)
    mzMLpath <- system.file("iontrap", package = "msdata")
    mzMLfiles<-list.files(mzMLpath, pattern = "extracted.mzML",
                          recursive = TRUE, full.names = TRUE)
    xs <- xcmsSet(mzMLfiles, 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 choosen method.

Methods

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

See Also

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

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

Description

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

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

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

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

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

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

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

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

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

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

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

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

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

addParams,addParams<-: getter and setter for the addParams slot of the object. This slot stores optional additional parameters to be passed to the identifyMajorPeaks and peakDetectionCWT 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'
snthresh(object)

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Arguments

snthresh	numeric(1) defining the signal to noise ratio cutoff.
verboseColumns	logical(1) whether additional peak meta data columns should be returned.
scales	Numeric defining the scales of the continuous wavelet transform (CWT).
nearbyPeak	logical(1) whether to include nearby peaks of major peaks.
peakScaleRange	numeric(1) defining the scale range of the peak (larger than 5 by default).
ampTh	numeric(1) defining the minimum required relative amplitude of the peak (ratio of the maximum of CWT coefficients).
minNoiseLevel	numeric(1) defining the minimum noise level used in computing the SNR.
ridgeLength	numeric(1) defining the minimum highest scale of the peak in 2-D CWT coefficient matrix.
peakThr	numeric(1) with the minimum absolute intensity (above baseline) of peaks to be picked. If provided, the smoothing Savitzky-Golay filter is used (in the MassSpecWavelet) package to estimate the local intensity.
tuneIn	logical(1) whther to tune in the parameter estimation of the detected peaks.

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

Details

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

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

Value

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

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

Slots

snthresh,verboseColumns,scales,nearbyPeak,peakScaleRange,ampTh,minNoiseLevel,ridgeLength,peakThr,tu
: See corresponding parameter 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 OnDiskMSnExp objects (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: findChromPeaks(), findChromPeaks-centWave, findChromPeaks-centWaveWithPredIso findChromPeaks-massifquant, findChromPeaks-matchedFilter

Examples

```
library(MSnbase)
## 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-mzML", package = "msdata"),
                     recursive = TRUE, full.names = TRUE)
fticr <- readMSData(fticrf[1], msLevel. = 1, mode = "onDisk")

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

head(chromPeaks(fticr))
```

---

findPeaks.addPredictedIsotopeFeatures-methods

Feature detection based on predicted isotope features for high resolution LC/MS data

---

Description

Peak density and wavelet based feature detection aiming at isotope peaks for high resolution LC/MS data in centroid mode

Arguments

object	xcmsSet object
ppm	maxmial tolerated m/z deviation in consecutive scans, in ppm (parts per million)
peakwidth	Chromatographic peak width, given as range (min,max) in seconds
prefilter	prefilter=c(k,I). Prefilter step for the first phase. Mass traces are only retained if they contain at least k peaks with intensity >= I.

mzCenterFun	Function to calculate the m/z center of the feature: wMean intensity weighted mean of the feature m/z values, mean mean of the feature m/z values, apex use m/z value at peak apex, wMeanApex3 intensity weighted mean of the m/z value at peak apex and the m/z value left and right of it, meanApex3 mean of the m/z value at peak apex and the m/z value left and right of it.
integrate	Integration method. If =1 peak limits are found through descent on the mexican hat filtered data, if =2 the descent is done on the real data. Method 2 is very accurate but prone to noise, while method 1 is more robust to noise but less exact.
mzdiff	minimum difference in m/z for peaks with overlapping retention times, can be negative to allow overlap
fitgauss	logical, if TRUE a Gaussian is fitted to each peak
scanrange	scan range to process
noise	optional argument which is useful for data that was centroided without any intensity threshold, centroids with intensity < noise are omitted from ROI detection
sleep	number of seconds to pause between plotting peak finding cycles
verbose.columns	logical, if TRUE additional peak meta data columns are returned
xcmsPeaks	peak list picked using the centWave algorithm with parameter verbose.columns set to TRUE (columns scmin and scmax needed)
snthresh	signal to noise ratio cutoff, definition see below.
maxcharge	max. number of the isotope charge.
maxiso	max. number of the isotope peaks to predict for each detected feature.
mzIntervalExtension	logical, if TRUE predicted isotope ROIs (regions of interest) are extended in the m/z dimension to increase the detection of low intensity and hence noisy peaks.

Details

This algorithm is most suitable for high resolution LC/{TOF,OrbiTrap,FTICR}-MS data in centroid mode. In the first phase of the method isotope ROIs (regions of interest) in the LC/MS map are predicted. In the second phase these mass traces are further analysed. Continuous wavelet transform (CWT) is used to locate chromatographic peaks on different scales. The resulting peak list and the given peak list (xcmsPeaks) are merged and redundant peaks are removed.

Value

A matrix with columns:

mz	weighted (by intensity) mean of peak m/z across scans
mzmin	m/z peak minimum
mzmax	m/z peak maximum
rt	retention time of peak midpoint
rtmin	leading edge of peak retention time

rtmax	trailing edge of peak retention time
into	integrated peak intensity
intb	baseline corrected integrated peak intensity
maxo	maximum peak intensity
sn	Signal/Noise ratio, defined as (maxo - baseline)/sd, where maxo is the maximum peak intensity, baseline the estimated baseline value and sd the standard deviation of local chromatographic noise.
egauss	RMSE of Gaussian fit

if verbose.columns is TRUE additionally :

mu	Gaussian parameter mu
sigma	Gaussian parameter sigma
h	Gaussian parameter h
f	Region number of m/z ROI where the peak was localised
dppm	m/z deviation of mass trace across scans in ppm
scale	Scale on which the peak was localised
scpos	Peak position found by wavelet analysis
scmin	Left peak limit found by wavelet analysis (scan number)
scmax	Right peak limit found by wavelet analysis (scan number)

Methods

object = "xcmsRaw" `findPeaks.centWave(object, ppm=25, peakwidth=c(20,50), prefilter=c(3,100), mzCenterFun="wMean", integrate=1, mzdiff=-0.001, fitgauss=FALSE, scanrange= numeric(), noise=0, sleep=0, verbose.columns=FALSE, xcmsPeaks, snthresh=6.25, maxcharge=3, maxiso=5, mzIntervalExtension=TRUE)`

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	maxmial tolerated m/z deviation in consecutive scans, in ppm (parts per million)
peakwidth	Chromatographic peak width, given as range (min,max) in seconds
snthresh	signal to noise ratio cutoff, definition see below.
prefilter	prefilter=c(k,I). Prefilter step for the first phase. Mass traces are only retained if they contain at least k peaks with intensity >= I.
mzCenterFun	Function to calculate the m/z center of the feature: wMean intensity weighted mean of the feature m/z values, mean mean of the feature m/z values, apex use m/z value at peak apex, wMeanApex3 intensity weighted mean of the m/z value at peak apex and the m/z value left and right of it, meanApex3 mean of the m/z value at peak apex and the m/z value left and right of it.
integrate	Integration method. If =1 peak limits are found through descent on the mexican hat filtered data, if =2 the descent is done on the real data. Method 2 is very accurate but prone to noise, while method 1 is more robust to noise but less exact.
mzdiff	minimum difference in m/z for peaks with overlapping retention times, can be negative to allow overlap
fitgauss	logical, if TRUE a Gaussian is fitted to each peak
scanrange	scan range to process
noise	optional argument which is useful for data that was centroided without any intensity threshold, centroids with intensity < noise are omitted from ROI detection
sleep	number of seconds to pause between plotting peak finding cycles
verbose.columns	logical, if TRUE additional peak meta data columns are returned
ROI.list	A optional list of ROIs that represents detected mass traces (ROIs). If this list is empty (default) then centWave detects the mass trace ROIs, otherwise this step is skipped and the supplied ROIs are used in the peak detection phase. Each ROI object in the list has the following slots: scmin start scan index, scmax end scan index, mzmin minimum m/z, mzmax maximum m/z, length number of scans, intensity summed intensity.
firstBaselineCheck	logical, if TRUE continuous data within ROI is checked to be above 1st baseline
roiScales	numeric, optional vector of scales for each ROI in ROI.list to be used for the centWave-wavelets

Details

This algorithm is most suitable for high resolution LC/{TOF,OrbiTrap,FTICR}-MS data in centroid mode. In the first phase of the method mass traces (characterised as regions with less than ppm m/z deviation in consecutive scans) in the LC/MS map are located. In the second phase these mass traces are further analysed. Continuous wavelet transform (CWT) is used to locate chromatographic peaks on different scales.

Value

A matrix with columns:

mz	weighted (by intensity) mean of peak m/z across scans
mzmin	m/z peak minimum
mzmax	m/z peak maximum
rt	retention time of peak midpoint
rtmin	leading edge of peak retention time
rtmax	trailing edge of peak retention time
into	integrated peak intensity
intb	baseline corrected integrated peak intensity
maxo	maximum peak intensity
sn	Signal/Noise ratio, defined as (maxo - baseline)/sd, where maxo is the maximum peak intensity, baseline the estimated baseline value and sd the standard deviation of local chromatographic noise.
egauss	RMSE of Gaussian fit

if verbose.columns is TRUE additionally :

mu	Gaussian parameter mu
sigma	Gaussian parameter sigma
h	Gaussian parameter h
f	Region number of m/z ROI where the peak was localised
dppm	m/z deviation of mass trace across scans in ppm
scale	Scale on which the peak was localised
scpos	Peak position found by wavelet analysis
scmin	Left peak limit found by wavelet analysis (scan number)
scmax	Right peak limit found by wavelet analysis (scan number)

Methods

object = "xcmsRaw" `findPeaks.centWave(object, ppm=25, peakwidth=c(20,50), snthresh=10, prefilter=c(3,100), mzCenterFun="wMean", integrate=1, mzdiff=-0.001, fitgauss=FALSE, scanrange= numeric(), noise=0, sleep=0, verbose.columns=FALSE, ROI.list=list()), firstBaselineCheck=TRUE, roiScales=NULL`

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

See Also

centWave for the new user interface. findPeaks-methods xcmsRaw-class

---

findPeaks.centWaveWithPredictedIsotopeROIs-methods

Feature detection with centWave and additional isotope features

---

Description

Peak density and wavelet based feature detection for high resolution LC/MS data in centroid mode with additional peak picking of isotope features on basis of isotope peak predictions

Arguments

object	xcmsSet object
ppm	maxmial tolerated m/z deviation in consecutive scans, in ppm (parts per million)
peakwidth	Chromatographic peak width, given as range (min,max) in seconds
snthresh	signal to noise ratio cutoff, definition see below.
prefilter	prefilter=c(k,I). Prefilter step for the first phase. Mass traces are only retained if they contain at least k peaks with intensity >= I.
mzCenterFun	Function to calculate the m/z center of the feature: wMean intensity weighted mean of the feature m/z values, mean mean of the feature m/z values, apex use m/z value at peak apex, wMeanApex3 intensity weighted mean of the m/z value at peak apex and the m/z value left and right of it, meanApex3 mean of the m/z value at peak apex and the m/z value left and right of it.
integrate	Integration method. If =1 peak limits are found through descent on the mexican hat filtered data, if =2 the descent is done on the real data. Method 2 is very accurate but prone to noise, while method 1 is more robust to noise but less exact.
mzdiff	minimum difference in m/z for peaks with overlapping retention times, can be negative to allow overlap
fitgauss	logical, if TRUE a Gaussian is fitted to each peak
scanrange	scan range to process
noise	optional argument which is useful for data that was centroided without any intensity threshold, centroids with intensity < noise are omitted from ROI detection

`sleep` number of seconds to pause between plotting peak finding cycles

`verbose.columns`
logical, if TRUE additional peak meta data columns are returned

`ROI.list` A optional list of ROIs that represents detected mass traces (ROIs). If this list is empty (default) then centWave detects the mass trace ROIs, otherwise this step is skipped and the supplied ROIs are used in the peak detection phase. Each ROI object in the list has the following slots: `scmin` start scan index, `scmax` end scan index, `mzmin` minimum m/z, `mzmax` maximum m/z, `length` number of scans, `intensity` summed intensity.

`firstBaselineCheck`
logical, if TRUE continuous data within ROI is checked to be above 1st baseline

`roiScales` numeric, optional vector of scales for each ROI in `ROI.list` to be used for the centWave-wavelets

`snthreshIsoROIs`
signal to noise ratio cutoff for predicted isotope ROIs, definition see below.

`maxcharge` max. number of the isotope charge.

`maxiso` max. number of the isotope peaks to predict for each detected feature.

`mzIntervalExtension`
logical, if TRUE predicted isotope ROIs (regions of interest) are extended in the m/z dimension to increase the detection of low intensity and hence noisy peaks.

Details

This algorithm is most suitable for high resolution LC/{TOF,OrbiTrap,FTICR}-MS data in centroid mode. The `centWave` algorithm is applied in two peak picking steps as follows. In the first peak picking step ROIs (regions of interest, characterised as regions with less than `ppm` m/z deviation in consecutive scans) in the LC/MS map are located and further analysed using continuous wavelet transform (CWT) for the localization of chromatographic peaks on different scales. In the second peak picking step isotope ROIs in the LC/MS map are predicted further analysed using continuous wavelet transform (CWT) for the localization of chromatographic peaks on different scales. The peak lists resulting from both peak picking steps are merged and redundant peaks are removed.

Value

A matrix with columns:

`mz` weighted (by intensity) mean of peak m/z across scans

`mzmin` m/z peak minimum

`mzmax` m/z peak maximum

`rt` retention time of peak midpoint

`rtmin` leading edge of peak retention time

`rtmax` trailing edge of peak retention time

`into` integrated peak intensity

`intb` baseline corrected integrated peak intensity

`maxo` maximum peak intensity

sn	Signal/Noise ratio, defined as (maxo - baseline)/sd, where maxo is the maximum peak intensity, baseline the estimated baseline value and sd the standard deviation of local chromatographic noise.
egauss	RMSE of Gaussian fit

if verbose.columns is TRUE additionally :

mu	Gaussian parameter mu
sigma	Gaussian parameter sigma
h	Gaussian parameter h
f	Region number of m/z ROI where the peak was localised
dppm	m/z deviation of mass trace across scans in ppm
scale	Scale on which the peak was localised
scpos	Peak position found by wavelet analysis
scmin	Left peak limit found by wavelet analysis (scan number)
scmax	Right peak limit found by wavelet analysis (scan number)

Methods

object = "xcmsRaw" `findPeaks.centWaveWithPredictedIsotopeROIs(object, ppm=25, peakwidth=c(20,50), snthresh=10, prefilter=c(3,100), mzCenterFun="wMean", integrate=1, mzdiff=-0.001, fitgauss=FALSE, scanrange= numeric(), noise=0, sleep=0, verbose.columns=FALSE, ROI.list=list(), firstBaselineCheck=TRUE, roiScales=NULL, snthreshIsoROIs=6.25, maxcharge=3, maxiso=5, mzIntervalExtension=TRUE)`

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.addPredictedIso
findPeaks.centWave findPeaks-methods xcmsRaw-class

`findPeaks.massifquant-methods`
Feature detection for XC-MS data.

Description

Massifquant is a Kalman filter (KF) based feature detection for XC-MS data in centroid mode (currently in experimental stage). Optionally allows for calling the method "centWave" on features discovered by Massifquant to further refine the feature detection; to do so, supply any additional parameters specific to centWave (even more experimental). The method may be conveniently called through the xcmsSet(...) method.

Arguments

The following arguments are specific to Massifquant. Any additional arguments supplied must correspond as specified by the method findPeaks.centWave.

`object`	An xcmsRaw object.
`criticalValue`	Numeric: Suggested values: (0.1-3.0). This setting helps determine the the Kalman Filter prediciton margin of error. A real centroid belonging to a bonafide feature must fall within the KF prediction margin of error. Much like in the construction of a confidence interval, criticalVal loosely translates to be a multiplier of the standard error of the prediction reported by the Kalman Filter. If the features in the XC-MS sample have a small mass deviance in ppm error, a smaller critical value might be better and vice versa.
`consecMissedLimit`	Integer: Suggested values:(1,2,3). While a feature is in the proces of being detected by a Kalman Filter, the Kalman Filter may not find a predicted centroid in every scan. After 1 or more consecutive failed predictions, this setting informs Massifquant when to stop a Kalman Filter from following a candidate feature.
`prefilter`	Numeric Vector: (Positive Integer, Positive Numeric): The first argument is only used if (withWave = 1); see centWave for details. The second argument specifies the minimum threshold for the maximum intensity of a feature that must be met.
`peakwidth`	Integer Vector: (Positive Integer, Positive Integer): Only the first argument is used for Massifquant, which specifices the minimum feature length in time scans. If centWave is used, then the second argument is the maximum feature length subject to being greater than the mininum feature length.
`ppm`	The minimum estimated parts per million mass resolution a feature must possess.
`unions`	Integer: set to 1 if apply t-test union on segmentation; set to 0 if no t-test to be applied on chromatographically continous features sharing same m/z range. Explanation: With very few data points, sometimes a Kalman Filter stops tracking a feature prematurely. Another Kalman Filter is instantiated and begins following the rest of the signal. Because tracking is done backwards to forwards, this algorithmic defect leaves a real feature divided into two segments or more. With

this option turned on, the program identifies segmented features and combines them (merges them) into one with a two sample t-test. The potential danger of this option is that some truly distinct features may be merged.

withWave — Integer: set to 1 if turned on; set to 0 if turned off. Allows the user to find features first with Massifquant and then filter those features with the second phase of centWave, which includes wavelet estimation.

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

Details

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

Value

If the method findPeaks.massifquant(...) is used, then a matrix is returned with rows corresponding to features, and properties of the features listed with the following column names. Otherwise, if centWave feature is used also (withWave = 1), or Massifquant is called through the xcmsSet(...) method, then their corresponding return values are used.

mz — weighted m/z mean (weighted by intensity) of the feature

mzmin — m/z lower boundary of the feature

mzmax — m/z upper boundary of the feature

rtmin — starting scan time of the feature

rtmax — starting scan time of the feature

into — the raw quantitation (area under the curve) of the feature.

area — feature area that is not normalized by the scan rate.

Methods

object = "xcmsRaw" `findPeaks.massifquant(object, ppm=10, peakwidth=c(20,50), snthresh=10, prefilter=c(3,100), mzCenterFun="wMean", integrate=1, mzdiff=-0.001, fitgauss=FALSE,`

```
scanrange= numeric(), noise=0, sleep=0, verbose.columns=FALSE, criticalValue =
1.125, consecMissedLimit = 2, unions = 1, checkBack = 0, withWave = 0)
```

Author(s)

Christopher Conley

References

Submitted for review. Christopher Conley, Ralf J .O Torgrip. Ryan Taylor, and John T. Prince. "Massifquant: open-source Kalman filter based XC-MS feature detection". August 2013.

See Also

centWave for the new user interface. findPeaks-methods xcmsSet xcmsRaw xcmsRaw-class

Examples

```
library(faahKO)
library(xcms)
#load all the wild type and Knock out samples
cdfpath <- system.file("cdf", package = "faahKO")
## Subset to only the first 2 files.
cdffiles <- list.files(cdfpath, recursive = TRUE, full.names = TRUE)[1:2]

## Run the massifquant analysis. Setting the noise level to 10000 to speed up
## execution of the examples - in a real use case it should be set to a reasoable
## value.
xset <- xcmsSet(cdffiles, method = "massifquant",
                consecMissedLimit = 1,
                snthresh = 10,
                criticalValue = 1.73,
                ppm = 10,
                peakwidth= c(30, 60),
                prefilter= c(1,3000),
                noise = 10000,
                withWave = 0)
```

---

findPeaks.matchedFilter,xcmsRaw-method

Peak detection in the chromatographic time domain

Description

Find peaks in the chromatographic time domain of the profile matrix. For more details see do_findChromPeaks_matchedFil

Usage

```
## S4 method for signature 'xcmsRaw'
findPeaks.matchedFilter(
  object,
  fwhm = 30,
  sigma = fwhm/2.3548,
  max = 5,
  snthresh = 10,
  step = 0.1,
  steps = 2,
  mzdiff = 0.8 - step * steps,
  index = FALSE,
  sleep = 0,
  scanrange = numeric()
)
```

Arguments

object	The xcmsRaw object on which peak detection should be performed.
fwhm	numeric(1) specifying the full width at half maximum of matched filtration gaussian model peak. Only used to calculate the actual sigma, see below.
sigma	numeric(1) specifying the standard deviation (width) of the matched filtration model peak.
max	numeric(1) representing the maximum number of peaks that are expected/will be identified per slice.
snthresh	numeric(1) defining the signal to noise cutoff to be used in the chromatographic peak detection step.
step	numeric(1) specifying the width of the bins/slices in m/z dimension.
steps	numeric(1) defining the number of bins to be merged before filtration (i.e. the number of neighboring bins that will be joined to the slice in which filtration and peak detection will be performed).
mzdiff	numeric(1) defining the minimum difference in m/z for peaks with overlapping retention times
index	logical(1) specifying whether indicies should be returned instead of values for m/z and retention times.
sleep	(DEPRECATED). The use of this parameter is highly discouraged, as it could cause problems in parallel processing mode.
scanrange	Numeric vector defining the range of scans to which the original object should be sub-setted before peak detection.

Value

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

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

mzmin Minimum m/z of the peak.

mzmax Maximum m/z of the peak.

rt Retention time of the peak's midpoint.

rtmin Minimum retention time of the peak.

rtmax Maximum retention time of the peak.

into Integrated (original) intensity of the peak.

intf Integrated intensity of the filtered peak.

maxo Maximum intensity of the peak.

maxf Maximum intensity of the filtered peak.

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

sn Signal to noise ratio of the peak.

Author(s)

Colin A. Smith

References

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

See Also

matchedFilter for the new user interface. xcmsRaw, do_findChromPeaks_matchedFilter for the core function performing the peak detection.

---

findPeaks.MS1-methods *Collecting MS1 precursor peaks*

Description

Collecting Tandem MS or MS^n Mass Spectrometry precursor peaks as annotated in XML raw file

Arguments

object	xcmsRaw object

Details

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

Since xcmsFragments attaches *all* MS^n peaks to MS1 peaks in xcmsSet, it is important that findPeaks and xcmsSet do not miss any MS1 precursor peak.

To be sure that all MS1 precursor peaks are in an xcmsSet, findPeaks.MS1 does not do an actual peak picking, but simply uses the annotation stored in mzXML, mzData or mzML raw files.

This relies on the following XML tags:

mzData: `<spectrum id="463"> <spectrumInstrument msLevel="2"> <cvParam cvLabel="psi" accession="PSI:1000039" name="TimeInSeconds" value="92.7743"/> </spectrumInstrument> <precursor msLevel="1" spectrumRef="461"> <cvParam cvLabel="psi" accession="PSI:1000040" name="MassToChargeRatio" value="462.091"/> <cvParam cvLabel="psi" accession="PSI:1000042" name="Intensity" value="366.674"/> </precursor> </spectrum>`

mzXML: `<scan num="17" msLevel="2" retentionTime="PT1.5224S"> <precursorMz precursorIntensity="125245" </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 `peakDetectionCWT` and `identifyMajorPeaks` functions from the `MassSpecWavelet` package.

Details

This is a wrapper around the peak picker in Bioconductor's `MassSpecWavelet` package calling `peakDetectionCWT` and `tuneInPeakInfo` functions.

Value

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

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

mzmin Minimum m/z of the peak.

mzmax Maximum m/z of the peak.

rt Always `-1`.

rtmin Always `-1`.

rtmax Always `-1`.

into Integrated (original) intensity of the peak.

maxo Maximum intensity of the peak.

intf Always `NA`.

maxf Maximum MSW-filter response of the peak.

sn Signal to noise ratio.

Author(s)

Joachim Kutzera, Steffen Neumann, Johannes Rainer

See Also

MSW for the new user interface, do_findPeaks_MSW for the downstream analysis function or peakDetectionCWT from the MassSpecWavelet for details on the algorithm and additionally supported parameters.

GenericParam-class *Generic parameter class*

Description

The GenericParam class allows to store generic parameter information such as the name of the function that was/has to be called (slot fun) and its arguments (slot args). This object is used to track the process history of the data processings of an XCMSnExp object. This is in contrast to e.g. the CentWaveParam object that is passed to the actual processing method.

Usage

```
GenericParam(fun = character(), args = list())
```

Arguments

fun	character representing the name of the function.
args	list (ideally named) with the arguments to the function.

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.

Author(s)

Johannes Rainer

See Also

processHistory for how to access the process history of an XCMSnExp object.

Examples

```
prm <- GenericParam(fun = "mean")

prm <- GenericParam(fun = "mean", args = list(na.rm = TRUE))
```

getEIC-methods *Get extracted ion chromatograms for specified m/z ranges*

Description

Generate multiple extracted ion chromatograms for m/z values of interest. For xcmsSet objects, reread original raw data and apply precomputed retention time correction, if applicable.

Note that this method will *always* return profile, not raw data (with profile data being the binned data along M/Z). See details for further information.

Arguments

object	the xcmsRaw or xcmsSet object
mzrange	Either a two column matrix with minimum or maximum m/z or a matrix of any dimensions containing columns mzmin and mzmax. If not specified, the method for xcmsRaw returns the base peak chromatogram (BPC, i.e. the most intense signal for each RT across all m/z). For xcmsSet objects the group data will be used if mzrange is not provided.
rtrange	A two column matrix the same size as mzrange with minimum and maximum retention times between which to return EIC data points. If not specified, the method returns the chromatogram for the full RT range. For xcmsSet objects, it may also be a single number specifying the time window around the peak to return EIC data points
step	step (bin) size to use for profile generation. Note that a value of step = 0 is not supported.
groupidx	either character vector with names or integer vector with indicies of peak groups for which to get EICs
sampleidx	either character vector with names or integer vector with indicies of samples for which to get EICs
rt	"corrected" for using corrected retention times, or "raw" for using raw retention times

Details

In contrast to the rawEIC method, that extracts the actual raw values, this method extracts them from the object's profile matrix (or if the provided step argument does not match the profStep of the object the profile matrix is calculated on the fly and the values returned).

Value

For xcmsSet and xcmsRaw objects, an xcmsEIC object.

Methods

object = "xcmsRaw" `getEIC(object, mzrange, rtrange = NULL, step = 0.1)`

object = "xcmsSet" `getEIC(object, mzrange, rtrange = 200, groupidx, sampleidx = sampnames(object), rt = c("corrected", "raw"))`

See Also

xcmsRaw-class, xcmsSet-class, xcmsEIC-class, rawEIC

---

getPeaks-methods *Get peak intensities for specified regions*

Description

Integrate extracted ion chromatograms in pre-defined defined regions. Return output similar to findPeaks.

Arguments

object	the xcmsSet object
peakrange	matrix or data frame with 4 columns: mzmin, mzmax, rtmin, rtmax (they must be in that order or named)
step	step size to use for profile generation

Value

A matrix with columns:

i	rank of peak identified in merged EIC (<= max), always NA
mz	weighted (by intensity) mean of peak m/z across scans
mzmin	m/z of minimum step
mzmax	m/z of maximum step
ret	retention time of peak midpoint
retmin	leading edge of peak retention time
retmax	trailing edge of peak retention time
into	integrated area of original (raw) peak
intf	integrated area of filtered peak, always NA
maxo	maximum intensity of original (raw) peak
maxf	maximum intensity of filtered peak, always NA

Methods

object = "xcmsRaw" `getPeaks(object, peakrange, step = 0.1)`

See Also

xcmsRaw-class

getScan-methods *Get m/z and intensity values for a single mass scan*

Description

Return the data from a single mass scan using the numeric index of the scan as a reference.

Arguments

object	the xcmsRaw object
scan	integer index of scan. if negative, the index numbered from the end
mzrange	limit data points returned to those between in the range, range(mzrange)

Value

A matrix with two columns:

mz	m/z values
intensity	intensity values

Methods

object = "xcmsRaw" getScan(object, scan, mzrange = numeric()) getMsnScan(object, scan, mzrange = numeric())

See Also

xcmsRaw-class, getSpec

getSpec-methods *Get average m/z and intensity values for multiple mass scans*

Description

Return full-resolution averaged data from multiple mass scans.

Arguments

object	the xcmsRaw object
...	arguments passed to profRange used to sepecify the spectral segments of interest for averaging

Details

Based on the mass points from the spectra selected, a master unique list of masses is generated. Every spectra is interpolated at those masses and then averaged.

Value

A matrix with two columns:

`mz`	m/z values
`intensity`	intensity values

Methods

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

See Also

`xcmsRaw-class`, `profRange`, `getScan`

`getXcmsRaw-methods` *Load the raw data for one or more files in the xcmsSet*

Description

Reads the raw data applies evential retention time corrections and waters Lock mass correction and returns it as an `xcmsRaw` object (or list of `xcmsRaw` objects) for one or more files of the `xcmsSet` object.

Arguments

`object`	the `xcmsSet` object
`sampleidx`	The index of the sample for which the raw data should be returned. Can be a single number or a numeric vector with the indices. Alternatively, the file name can be specified.
`profmethod`	The profile method.
`profstep`	The profile step.
`rt`	Whether corrected or raw retention times should be returned.
`...`	Additional arguments submitted to the `xcmsRaw` function.

Value

A single `xcmsRaw` object or a list of `xcmsRaw` objects.

Methods

object = "xcmsSet" `getXcmsRaw(object, sampleidx=1, profmethod=profinfo(object)$method, profstep=profinfo(object)$step, rt=c("corrected", "raw"), ... )`

Author(s)

Johannes Rainer, <johannes.rainer@eurac.edu>

See Also

xcmsRaw-class,

---

group-methods *Group peaks from different samples together*

Description

A number of grouping (or alignment) methods exist in XCMS. group is the generic method.

Arguments

object	xcmsSet-class object
method	Method to use for grouping. See details.
...	Optional arguments to be passed along

Details

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

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

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

Value

An xcmsSet object with peak group assignments and statistics.

Methods

object = "xcmsSet" group(object, ...)

See Also

group.density group.mzClust group.nearest xcmsSet-class,

group.density *Group peaks from different samples together*

Description

Group peaks together across samples using overlapping m/z bins and calculation of smoothed peak distributions in chromatographic time.

Arguments

object	the xcmsSet object
minfrac	minimum fraction of samples necessary in at least one of the sample groups for it to be a valid group
minsamp	minimum number of samples necessary in at least one of the sample groups for it to be a valid group
bw	bandwidth (standard deviation or half width at half maximum) of gaussian smoothing kernel to apply to the peak density chromatogram
mzwid	width of overlapping m/z slices to use for creating peak density chromatograms and grouping peaks across samples
max	maximum number of groups to identify in a single m/z slice
sleep	seconds to pause between plotting successive steps of the peak grouping algorithm. peaks are plotted as points showing relative intensity. identified groups are flanked by dotted vertical lines.

Value

An xcmsSet object with peak group assignments and statistics.

Methods

object = "xcmsSet" `group(object, bw = 30, minfrac = 0.5, minsamp = 1, mzwid = 0.25, max = 50, sleep = 0)`

See Also

`do_groupChromPeaks_density` for the core API function performing the analysis. `xcmsSet-class`, `density`

group.mzClust *Group Peaks via High Resolution Alignment*

Description

Runs high resolution alignment on single spectra samples stored in a given xcmsSet.

Arguments

object	a xcmsSet with peaks
mzppm	the relative error used for clustering/grouping in ppm (parts per million)
mzabs	the absolute error used for clustering/grouping
minsamp	set the minimum number of samples in one bin
minfrac	set the minimum fraction of each class in one bin

Value

Returns a xcmsSet with slots groups and groupindex set.

Methods

object = "xcmsSet" `group(object, method="mzClust", mzppm = 20, mzabs = 0, minsamp = 1, minfrac=0)`

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)
mzMLpath <- system.file("fticr-mzML", package = "msdata")
mzMLfiles <- list.files(mzMLpath, recursive = TRUE, full.names = TRUE)

xs <- xcmsSet(method="MSW", files=mzMLfiles, 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")
    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(object)) ))
                               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 ## number of features after minFrac

## End(Not run)
```

---

groupChromPeaks *Correspondence: group chromatographic peaks across samples*

Description

The groupChromPeaks method performs a correspondence analysis i.e., it groups chromatographic peaks across samples to define the LC-MS *features*. The correspondence algorithm can be selected, and configured, using the param argument. See documentation of XcmsExperiment() and XCMSnExp() for information on how to access and extract correspondence results.

The correspondence analysis can be performed on chromatographic peaks of any MS level (if present and if chromatographic peak detection has been performed for that MS level) defining features combining these peaks. The MS level can be selected with the parameter msLevel. By default, calling groupChromPeaks will remove any previous correspondence results. This can be disabled with add = TRUE, which will add newly defined features to already present feature definitions.

Supported param objects are:

- PeakDensityParam: correspondence using the *peak density* method (Smith 2006) that groups chromatographic peaks along the retention time axis within slices of (partially overlapping) m/z ranges. By default, these m/z ranges (bins) have a constant size. By setting ppm to a value larger than 0, m/z dependent bin sizes can be used instead (better representing the m/z

dependent measurement error of some MS instruments). All peaks (from the same or from different samples) with their apex position being close on the retention time axis are grouped into a LC-MS feature. See in addition `do_groupChromPeaks_density()` for the core API function.

- `NearestPeaksParam`: performs peak grouping based on the proximity of chromatographic peaks from different samples in the m/z - rt space similar to the correspondence method of *mzMine* (Katajamaa 2006). The method creates first a *master peak list* consisting of all chromatographic peaks from the sample with the most detected peaks and iteratively calculates distances to peaks from the sample with the next most number of peaks grouping peaks together if their *distance* is smaller than the provided thresholds. See in addition `do_groupChromPeaks_nearest()` for the core API function.
- `MzClustParam`: performs high resolution peak grouping for **single spectrum** metabolomics data (Kazmi 2006). This method should **only** be used for such data as the retention time is not considered in the correspondence analysis. See in addition `do_groupPeaks_mzClust()` for the core API function.

For specific examples and description of the method and settings see the help pages of the individual parameter classes listed above.

Usage

```
groupChromPeaks(object, param, ...)

## S4 method for signature 'XcmsExperiment,Param'
groupChromPeaks(object, param, msLevel = 1L, add = FALSE)

PeakDensityParam(
  sampleGroups = numeric(),
  bw = 30,
  minFraction = 0.5,
  minSamples = 1,
  binSize = 0.25,
  ppm = 0,
  maxFeatures = 50
)

MzClustParam(
  sampleGroups = numeric(),
  ppm = 20,
  absMz = 0,
  minFraction = 0.5,
  minSamples = 1
)

NearestPeaksParam(
  sampleGroups = numeric(),
  mzVsRtBalance = 10,
  absMz = 0.2,
  absRt = 15,
```

```
  kNN = 10
)

## 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 'PeakDensityParam'
ppm(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 '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 'PeakDensityParam'
as.list(x, ...)

## S4 method for signature 'XCMSnExp,PeakDensityParam'
groupChromPeaks(object, param, msLevel = 1L, add = FALSE)

## S4 method for signature 'XCMSnExp,MzClustParam'
groupChromPeaks(object, param, msLevel = 1L)

## S4 method for signature 'XCMSnExp,NearestPeaksParam'
groupChromPeaks(object, param, msLevel = 1L, add = FALSE)
```

Arguments

object	The data object on which the correspondence analysis should be performed. Can be an XCMSnExp(), XcmsExperiment() object.
param	The parameter object selecting and configuring the algorithm.
...	Optional parameters.
msLevel	integer(1) defining the MS level on which the chromatographic peak detection should be performed.
add	logical(1) (if object contains already chromatographic peaks, i.e. is either an XCMSnExp or XcmsExperiment) whether chromatographic peak detection results should be **added** to existing results. By default (add = FALSE) any additional findChromPeaks call on a result object will remove previous results.
sampleGroups	For PeakDensityParam: A vector of the same length than samples defining the sample group assignments (i.e. which samples belong to which sample group). This parameter is mandatory for the PeakDensityParam and has to be provided also if there is no sample grouping in the experiment (in which case all samples should be assigned to the same group).
bw	For PeakDensityParam: numeric(1) defining the bandwidth (standard deviation ot the smoothing kernel) to be used. This argument is passed to the [density() method.
minFraction	For PeakDensityParam: 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	For PeakDensityParam: 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	For PeakDensityParam: numeric(1) defining the size of the overlapping slices in m/z dimension.

ppm	For MzClustParam: numeric(1) representing the relative m/z error for the clustering/grouping (in parts per million). For PeakDensityParam: numeric(1) to define m/z-dependent, increasing m/z bin sizes. If ppm = 0 (the default) m/z bins are defined by the sequence of values from the smallest to the larges m/z value with a constant bin size of binSize. For ppm > 0 the size of each bin is increased in addition by the ppm of the (upper) m/z boundary of the bin. The maximal bin size (used for the largest m/z values) would then be binSize plus ppm parts-per-million of the largest m/z value of all peaks in the data set.
maxFeatures	For PeakDensityParam: numeric(1) with the maximum number of peak groups to be identified in a single mz slice.
absMz	For NearestPeaksParam and MzClustParam: numeric(1) maximum tolerated distance for m/z values.
mzVsRtBalance	For NearestPeaksParam: numeric(1) representing the factor by which m/z values are multiplied before calculating the (euclician) distance between two peaks.
absRt	For NearestPeaksParam: numeric(1) maximum tolerated distance for retention times.
kNN	For NearestPeaksParam: integer(1) representing the number of nearest neighbors to check.
value	The value for the slot.
x	The parameter object.

Value

For groupChromPeaks: either an XcmsExperiment() or XCMSnExp() object with the correspondence result.

Author(s)

Colin Smith, Johannes Rainer

References

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

Kazmi S. A., Ghosh, S., Shin, D., Hill, D.W., and Grant, D.F. (2006) "Alignment of high resolution mass spectra: development of a heuristic approach for metabolomics. *Metabolomics* Vol. 2, No. 2, 75-83.

groupFeatures-abundance-correlation

Compounding/feature grouping based on similarity of abundances across samples

Description

Features from the same originating compound are expected to have similar intensities across samples. This method thus groups features based on similarity of abundances (i.e. *feature values*) across samples in a data set. See also AbundanceSimilarityParam() for additional information and details.

This help page lists parameters specific for xcms result objects (i.e. XcmsExperiment() and XCMSnExp() objects). Documentation of the parameters for the similarity calculation is available in the AbundanceSimilarityParam() help page in the MsFeatures package.

Usage

```
## S4 method for signature 'XcmsResult,AbundanceSimilarityParam'
groupFeatures(
  object,
  param,
  msLevel = 1L,
  method = c("medret", "maxint", "sum"),
  value = "into",
  intensity = "into",
  filled = TRUE,
  ...
)
```

Arguments

object	XcmsExperiment() or XCMSnExp() object containing LC-MS pre-processing results.
param	AbudanceSimilarityParam object with the settings for the method. See AbundanceSimilarityParam() for details on the grouping method and its parameters.
msLevel	integer(1) defining the MS level on which the features should be grouped.
method	character(1) passed to the featureValues call. See featureValues() for details. Defaults to method = "medret".
value	character(1) passed to the featureValues call. See featureValues() for details. Defaults to value = "into".
intensity	character(1) passed to the featureValues call. See featureValues() for details. Defaults to intensity = "into".
filled	logical(1) whether filled-in values should be included in the correlation analysis. Defaults to filled = TRUE.
...	additional parameters passed to the groupFeatures method for matrix.

Value

input object with feature group definitions added to (or updated in) a column "feature_group" in its featureDefinitions data frame.

Author(s)

Johannes Rainer

See Also

feature-grouping for a general overview.

Other feature grouping methods: groupFeatures-eic-similarity, groupFeatures-similar-rtime

Examples

```
library(MsFeatures)
library(MsExperiment)
## Load a test data set with detected peaks
faahko_sub <- loadXcmsData("faahko_sub2")

## Disable parallel processing for this example
register(SerialParam())

## Group chromatographic peaks across samples
xodg <- groupChromPeaks(faahko_sub, param = PeakDensityParam(sampleGroups = rep(1, 3)))

## Group features based on correlation of feature values (integrated
## peak area) across samples. Note that there are many missing values
## in the feature value which influence grouping of features in the present
## data set.
xodg_grp <- groupFeatures(xodg,
    param = AbundanceSimilarityParam(threshold = 0.8))
table(featureDefinitions(xodg_grp)$feature_group)

## Group based on the maximal peak intensity per feature
xodg_grp <- groupFeatures(xodg,
    param = AbundanceSimilarityParam(threshold = 0.8, value = "maxo"))
table(featureDefinitions(xodg_grp)$feature_group)
```

---

groupFeatures-eic-similarity

Compounding/feature grouping based on similarity of extracted ion chromatograms

---

Description

Features from the same originating compound are expected to share their elution pattern (i.e. chromatographic peak shape) with it. Thus, this methods allows to group features based on similarity of their extracted ion chromatograms (EICs). The similarity calculation is performed separately for each sample with the similarity score being aggregated across samples for the final generation of the similarity matrix on which the grouping (considering parameter `threshold`) will be performed.

The `compareChromatograms()` function is used for similarity calculation which by default calculates the Pearson's correlation coefficient. The settings for `compareChromatograms` can be specified with parameters `ALIGNFUN`, `ALIGNFUNARGS`, `FUN` and `FUNARGS`. `ALIGNFUN` defaults to `alignRt()` and is the function used to *align* the chromatograms before comparison. `ALIGNFUNARGS` allows to specify additional arguments for the `ALIGNFUN` function. It defaults to `ALIGNFUNARGS = list(tolerance = 0, method = "closest")` which ensures that data points from the same spectrum (scan, i.e. with the same retention time) are compared between the EICs from the same sample. Parameter `FUN` defines the function to calculate the similarity score and defaults to `FUN = cor` and `FUNARGS` allows to pass additional arguments to this function (defaults to `FUNARGS = list(use = "pairwise.complete.obs")`. See also `compareChromatograms()` for more information.

The grouping of features based on the EIC similarity matrix is performed with the function specified with parameter `groupFun` which defaults to `groupFun = groupSimilarityMatrix` which groups all rows (features) in the similarity matrix with a similarity score larger than `threshold` into the same cluster. This creates clusters of features in which **all** features have a similarity score `>= threshold` with **any** other feature in that cluster. See `groupSimilarityMatrix()` for details. Additional parameters to that function can be passed with the `...` argument.

This feature grouping should be called **after** an initial feature grouping by retention time (see `SimilarRtimeParam()`). The feature groups defined in columns `"feature_group"` of `featureDefinitions(object)` (for features matching `msLevel`) will be used and refined by this method. Features with a value of `NA` in `featureDefinitions(object)$feature_group` will be skipped/not considered for feature grouping.

Usage

```
EicSimilarityParam(
  threshold = 0.9,
  n = 1,
  onlyPeak = TRUE,
  value = c("maxo", "into"),
  groupFun = groupSimilarityMatrix,
  ALIGNFUN = alignRt,
  ALIGNFUNARGS = list(tolerance = 0, method = "closest"),
  FUN = cor,
  FUNARGS = list(use = "pairwise.complete.obs"),
  ...
)

## S4 method for signature 'XcmsResult,EicSimilarityParam'
groupFeatures(object, param, msLevel = 1L)
```

Arguments

threshold	numeric(1) with the minimal required similarity score to group featues. This is passed to the groupFun function.
n	numeric(1) defining the total number of samples per feature group on which this similarity calculation should be performed. This value is rounded up to the next larger integer value.
onlyPeak	logical(1) whether the correlation should be performed only on the signals within the identified chromatographic peaks (onlyPeak = TRUE, default) or all the signal from the extracted ion chromatogram.
value	character(1) defining whether samples should be grouped based on the sum of the maximal peak intensity (value = "maxo", the default) or the integrated peak area (value = "into") for a feature.
groupFun	function defining the function to be used to group rows based on a pairwise similarity matrix. Defaults to groupSimilarityMatrix().
ALIGNFUN	function defining the function to be used to *align* chromatograms prior similarity calculation. Defaults to ALIGNFUN = alignRt. See alignRt() and compareChromatograms() for more information.
ALIGNFUNARGS	**named** list with arguments for ALIGNFUN. Defaults to ALIGNFUNARGS = list(tolerance = 0, method = "closest").
FUN	function defining the function to be used to calculate a similarity between (aligned) chromatograms. Defaults to FUN = cor. See cor() and compareChromatograms() for more information.
FUNARGS	**named** list with arguments for FUN. Defaults to FUN = list(use = "pairwise.complete.obs").
...	for EicSimilarityParam: additional arguments to be passed to groupFun and featureChromatograms (such as expandRt to expand the retention time range of each feature).
object	XcmsExperiment() or XCMSnExp() object with LC-MS pre-processing results.
param	EicSimilarityParam object with the settings for the method.
msLevel	integer(1) defining the MS level on which the features should be grouped.

Value

input object with feature groups added (i.e. in column "feature_group" of its featureDefinitions data frame.

Note

At present the featureChromatograms() function is used to extract the EICs for each feature, which does however use one m/z and rt range for each feature and the EICs do thus not exactly represent the identified chromatographic peaks of each sample (i.e. their specific m/z and retention time ranges).

While being possible to be performed on the full data set without prior feature grouping, this is not suggested for the following reasons: I) the selection of the top n samples with the highest signal for the *feature group* will be biased by very abundant compounds as this is performed on the full data

set (i.e. the samples with the highest overall intensities are used for correlation of all features) and II) it is computationally much more expensive because a pairwise correlation between all features has to be performed.

It is also suggested to perform the correlation on a subset of samples per feature with the highest intensities of the peaks (for that feature) although it would also be possible to run the correlation on all samples by setting `n` equal to the total number of samples in the data set. EIC correlation should however be performed ideally on samples in which the original compound is highly abundant to avoid correlation of missing values or noisy peak shapes as much as possible.

By default also the signal which is outside identified chromatographic peaks is excluded from the correlation.

Author(s)

Johannes Rainer

See Also

feature-grouping for a general overview.

Other feature grouping methods: `groupFeatures-abundance-correlation`, `groupFeatures-similar-rtime`

Examples

```
library(MsFeatures)
library(MsExperiment)
## Load a test data set with detected peaks
faahko_sub <- loadXcmsData("faahko_sub2")

## Disable parallel processing for this example
register(SerialParam())

## Group chromatographic peaks across samples
xodg <- groupChromPeaks(faahko_sub, param = PeakDensityParam(sampleGroups = rep(1, 3)))

## Performing a feature grouping based on EIC similarities on a single
## sample
xodg_grp <- groupFeatures(xodg, param = EicSimilarityParam(n = 1))

table(featureDefinitions(xodg_grp)$feature_group)

## Usually it is better to perform this correlation on pre-grouped features
## e.g. based on similar retention time.
xodg_grp <- groupFeatures(xodg, param = SimilarRtimeParam(diffRt = 4))
xodg_grp <- groupFeatures(xodg_grp, param = EicSimilarityParam(n = 1))

table(featureDefinitions(xodg_grp)$feature_group)
```

groupFeatures-similar-rtime *Compounding/feature grouping based on similar retention times*

Description

Group features based on similar retention time. This method is supposed to be used as an initial *crude* grouping of features based on the median retention time of all their chromatographic peaks. All features with a difference in their retention time which is <= parameter `diffRt` of the parameter object are grouped together. If a column `"feature_group"` is found in `featureDefinitions()` this is further sub-grouped by this method.

See `MsFeatures::SimilarRtimeParam()` in `MsFeatures` for more details.

Usage

```
## S4 method for signature 'XcmsResult,SimilarRtimeParam'
groupFeatures(object, param, msLevel = 1L, ...)
```

Arguments

`object`	`XcmsExperiment()` or `XCMSnExp()` object containing also correspondence results.
`param`	`SimilarRtimeParam` object with the settings for the method. See `MsFeatures::SimilarRtimeParam()` for details and options.
`msLevel`	`integer(1)` defining the MS level on which the features should be grouped.
`...`	passed to the `groupFeatures` function on numeric values.

Value

the input object with feature groups added (i.e. in column `"feature_group"` of its `featureDefinitions` data frame.

Author(s)

Johannes Rainer

See Also

Other feature grouping methods: `groupFeatures-abundance-correlation`, `groupFeatures-eic-similarity`

Examples

```
library(MsFeatures)
library(MsExperiment)
## Load a test data set with detected peaks
faahko_sub <- loadXcmsData("faahko_sub2")
```

```
## Disable parallel processing for this example
register(SerialParam())

## Group chromatographic peaks across samples
xodg <- groupChromPeaks(faahko_sub, param = PeakDensityParam(sampleGroups = rep(1, 3)))

## Group features based on similar retention time (i.e. difference <= 2 seconds)
xodg_grp <- groupFeatures(xodg, param = SimilarRtimeParam(diffRt = 2))

## Feature grouping get added to the featureDefinitions in column "feature_group"
head(featureDefinitions(xodg_grp)$feature_group)

table(featureDefinitions(xodg_grp)$feature_group)
length(unique(featureDefinitions(xodg_grp)$feature_group))

## Using an alternative groupiing method that creates larger groups
xodg_grp <- groupFeatures(xodg,
    param = SimilarRtimeParam(diffRt = 2, groupFun = MsCoreUtils::group))

length(unique(featureDefinitions(xodg_grp)$feature_group))
```

`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 unque names for peak groups*

Description

Allow linking of peak group data between classes using unique group names that remain the same as long as no re-grouping occurs.

Arguments

`object`	the `xcmsSet` or `xcmsEIC` object
`mzdec`	number of decimal places to use for m/z
`rtdec`	number of decimal places to use for retention time
`template`	a character vector with existing group names whose format should be emulated

Value

A character vector with unique names for each peak group in the object. The format is `M[m/z]T[time in seconds]`.

Methods

object = "xcmsSet" `(object, mzdec = 0, rtdec = 0, template = NULL)`

object = "xcmsEIC" `(object)`

See Also

`xcmsSet-class`, `xcmsEIC-class`

`groupOverlaps` *Group overlapping ranges*

Description

`groupOverlaps` identifies overlapping ranges in the input data and groups them by returning their indices in `xmin` `xmax`.

Usage

```
groupOverlaps(xmin, xmax)
```

Arguments

xmin	numeric (same length than xmax) with the lower boundary of the range.
xmax	numeric (same length than xmin) with the upper boundary of the range.

Value

list with the indices of grouped elements.

Author(s)

Johannes Rainer

Examples

```
x <- c(2, 12, 34.2, 12.4)
y <- c(3, 16, 35, 36)

groupOverlaps(x, y)
```

---

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", intensity = "into")`

See Also

xcmsSet-class

---

highlightChromPeaks *Add definition of chromatographic peaks to an extracted chromatogram plot*

Description

The highlightChromPeaks function adds chromatographic peak definitions to an existing plot, such as one created by the plot method on a Chromatogram or MChromatograms object.

Usage

```
highlightChromPeaks(
  x,
  rt,
  mz,
  peakIds = character(),
  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.
peakIds	character defining the IDs (i.e. rownames of the peak in the chromPeaks table) of the chromatographic peaks to be highlighted in a plot.
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 grapics 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

```
## Load a test data set with detected peaks
library(MSnbase)
data(faahko_sub)
## Update the path to the files for the local system
dirname(faahko_sub) <- system.file("cdf/KO", package = "faahKO")

## Disable parallel processing for this example
register(SerialParam())

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

plot(chrs)

## Extract chromatographic peaks for the mz/rt range (if any).
chromPeaks(faahko_sub, rt = c(2700, 2900), mz = 335)

## Highlight the chromatographic peaks in the area
## Show the peak definition with a rectangle
highlightChromPeaks(faahko_sub, rt = c(2700, 2900), mz = 335)

## Color the actual peak
highlightChromPeaks(faahko_sub, 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

x	A numeric vector with eventual missing (NA) values.
baseValue	The base value to which empty elements should be set. This is only considered for method = "linbase" and corresponds to the profBinLinBase's baselevel argument.
method	One of "none", "lin" or "linbase".
distance	For method = "linbase": number of non-empty neighboring element of an empty element that should be considered for linear interpolation. See details section for more information.
noInterpolAtEnds	For method = "lin": Logical indicating whether linear interpolation should also be performed at the ends of the data vector (i.e. if missing values are present at the beginning or the end of the vector).

Details

Values for NAs in input vector x can be imputed using methods "lin" and "linbase":

impute = "lin" uses simple linear imputation to derive a value for an empty element in input vector x from its neighboring non-empty elements. This method is equivalent to the linear interpolation in the profBinLin method. Whether interpolation is performed if missing values are present at the beginning and end of x can be set with argument noInterpolAtEnds. By default interpolation is also performed at the ends interpolating from 0 at the beginning and towards 0 at the end. For noInterpolAtEnds = TRUE no interpolation is performed at both ends replacing the missing values at the beginning and/or the end of x with 0.

impute = "linbase" uses linear interpolation to impute values for empty elements within a user-definable proximity to non-empty elements and setting the element's value to the baseValue otherwise. The default for the baseValue is half of the smallest value in x (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, it's vale is set to baseValue. This corresponds to the linear interpolation performed by the profBinLinBase method. For more details see examples below.

Value

A numeric vector with empty values imputed based on the selected method.

Author(s)

Johannes Rainer

Examples

```
#######
## Impute missing values by linearly interpolating from neighboring
```

```
## non-empty elements
x <- c(3, NA, 1, 2, NA, NA, 4, NA, NA, NA, 3, NA, NA, NA, NA, 2)
imputeLinInterpol(x, method = "lin")
## visualize the interpolation:
plot(x = 1:length(x), y = x)
points(x = 1:length(x), y = imputeLinInterpol(x, method = "lin"), type = "l", col = "grey")

## If the first or last elements are NA, interpolation is performed from 0
## to the first non-empty element.
x <- c(NA, 2, 1, 4, NA)
imputeLinInterpol(x, method = "lin")
## visualize the interpolation:
plot(x = 1:length(x), y = x)
points(x = 1:length(x), y = imputeLinInterpol(x, method = "lin"), type = "l", col = "grey")

## If noInterpolAtEnds is TRUE no interpolation is performed at both ends
imputeLinInterpol(x, method = "lin", noInterpolAtEnds = TRUE)

######
## method = "linbase"
## "linbase" performs imputation by interpolation for empty elements based on
## 'distance' adjacent non-empty elements, setting all remaining empty elements
## to the baseValue
x <- c(3, NA, 1, 2, NA, NA, 4, NA, NA, NA, 3, NA, NA, NA, NA, 2)
## Setting distance = 0 skips imputation by linear interpolation
imputeLinInterpol(x, method = "linbase", distance = 0)

## With distance = 1 for all empty elements next to a non-empty element the value
## is imputed by linear interpolation.
xInt <- imputeLinInterpol(x, method = "linbase", distance = 1L)
xInt

plot(x = 1:length(x), y = x, ylim = c(0, max(x, na.rm = TRUE)))
points(x = 1:length(x), y = xInt, type = "l", col = "grey")

## Setting distance = 2L would cause that for all empty elements for which the
## distance to the next non-empty element is <= 2 the value is imputed by
## linear interpolation:
xInt <- imputeLinInterpol(x, method = "linbase", distance = 2L)
xInt

plot(x = 1:length(x), y = x, ylim = c(0, max(x, na.rm = TRUE)))
points(x = 1:length(x), y = xInt, type = "l", col = "grey")
```

`imputeRowMin` *Replace missing values with a proportion of the row minimum*

Description

`imputeRowMin` imputes missing values in `x` by replacing `NA`s 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

x	matrix with abundances, rows being features/metabolites and columns samples.
min_fraction	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(MSnbase)
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 mimimum
head(imputeRowMin(mat, min_fraction = 1/8))
```

---

imputeRowMinRand *Impute missing values with random numbers based on the row minimum*

Description

Replace missing values with random numbers. When using the method = "mean_sd", random numbers will be generated 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. When using the method method = "from_to", random numbers between 2 specific values will be generated.

Usage

```
imputeRowMinRand(
  x,
  method = c("mean_sd", "from_to"),
  min_fraction = 1/2,
  min_fraction_from = 1/1000,
  sd_fraction = 1,
  abs = TRUE
)
```

Arguments

x	matrix with abundances, rows being features/metabolites and columns samples.
method	method character(1) defining the imputation method. See description for details. Defaults to method = "mean_sd".
min_fraction	numeric(1) with the fraction of the row minimum that should be used to replace NA values in that row in case that mean_sd method is specified. When using from_to method, this value will be the one used to calculate the maximum value for replace NA values in that row.
min_fraction_from	numeric(1) with the fraction of the row minimum that should be used to calculate the minimum value for replace NA values in that row. This parameter is used only in case that from_to method is specified.
sd_fraction	numeric(1) factor to reduce the estimated standard deviation. This parameter is used only in case that mean_sd method is specified.
abs	logical(1) to force imputed values to be strictly positive.

Details

For method **mean_sd**, 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.

For method **from_to**, imputed values are taken between 2 user defined fractions of the row minimum.

Author(s)

Johannes Rainer, Mar Garcia-Aloy

See Also

imputeLCMD package for more left censored imputation functions.

Other imputation functions: imputeRowMin()

Examples

```
library(faahKO)
library(MSnbase)
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_meansd <- imputeRowMinRand(mat, method = "mean_sd")
mat_imp_fromto <- imputeRowMinRand(mat, method = "from_to")

head(mat)
head(mat_imp_meansd)
head(mat_imp_fromto)
```

---

isolationWindowTargetMz,OnDiskMSnExp-method

Extract isolation window target m/z definition

Description

`isolationWindowTargetMz` extracts the isolation window target m/z definition for each spectrum in `object`.

Usage

```
## S4 method for signature 'OnDiskMSnExp'
isolationWindowTargetMz(object)
```

Arguments

`object`	OnDiskMSnExp object.

Value

a `numeric` of length equal to the number of spectra in `object` with the isolation window target m/z or `NA` if not specified/available.

Author(s)

Johannes Rainer

levelplot-methods *Plot log intensity image of a xcmsRaw object*

Description

Create an image of the raw (profile) data m/z against retention time, with the intensity color coded.

Arguments

x	xcmsRaw object.
log	Whether the intensity should be log transformed.
col.regions	The color ramp that should be used for encoding of the intensity.
rt	wheter the original (rt="raw") or the corrected (rt="corrected") retention times should be used.
...	Arguments for profRange.

Methods

x = "xcmsRaw" `levelplot(x, log=TRUE, col.regions=colorRampPalette(brewer.pal(9, "YlOrRd"))(256), ...)`

x = "xcmsSet" `levelplot(x, log=TRUE, col.regions=colorRampPalette(brewer.pal(9, "YlOrRd"))(256), rt="raw", ...)`

Author(s)

Johannes Rainer, <johannes.rainer@eurac.edu>

See Also

xcmsRaw-class, xcmsSet-class

loadRaw-methods *Read binary data from a source*

Description

This function extracts the raw data which will be used an xcmsRaw object. Further processing of data is done in the xcmsRaw constructor.

Arguments

object	Specification of a data source (such as a file name or database query)

Details

The implementing methods decide how to gather the data.

Value

A list containing elements describing the data source. The `rt`, `scanindex`, `tic`, and `acquisitionNum` components each have one entry per scan. They are *parallel* in the sense that `rt[1]`, `scanindex[1]`, and `acquisitionNum[1]` all refer to the same scan. The list containst the following components:

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

Methods

`signature(object = "xcmsSource")` Uses `loadRaw,xcmsSource-method` to extract raw data. Subclasses of `xcmsSource` can provide different ways of fetching data.

Author(s)

Daniel Hackney, <dan@haxney.org>

See Also

`xcmsRaw-class`, `xcmsSource`

`loadXcmsData` *LC-MS preprocessing result test data sets*

Description

Data sets with ‘xcms‘ preprocessing results are provided within the ‘xcms‘ package and can be loaded with the ‘loadXcmsData‘ function. The available Test data sets are:

- ‘xdata‘: an [XCMSnExp()] object with the results from a ‘xcms‘-based pre-processing of an LC-MS untargeted metabolomics data set. The raw data files are provided in the ‘faahKO‘ R package.

- ‘xmse‘: an [XcmsExperiment()] object with the results from an ‘xcms‘-based pre-processing of an LC-MS untargeted metabolomics data set (same original data set and pre-processing settings as for the ‘xdata‘ data set). The pre-processing of this data set is described in detail in the *xcms* vignette of the ‘xcms‘ package.

- 'faahko_sub': an [XCMSnExp()] object with identified chromatographic peaks in 3 samples from the data files in the 'faahKO' R package.

- 'faahko_sub2': an [XcmsExperiment()] object with identified chromatographic peaks in 3 samples from the data files in the 'faahKO' R package.

Data sets can also be loaded using 'data', which would however require to update objects to point to the location of the raw data files. The 'loadXcmsData' loads the data and ensures that all paths are updated accordingly.

Usage

```
loadXcmsData(x = c("xmse", "xdata", "faahko_sub", "faahko_sub2"))
```

Arguments

x	For 'loadXcmsData': 'character(1)' with the name of the data file (object) to load.

Examples

```
library(xcms)
xdata <- loadXcmsData()
```

---

manualChromPeaks *Manual peak integration and feature definition*

Description

The manualChromPeaks function allows to *manually* define chromatographic peaks, integrate the intensities within the specified peak area and add them to the object's chromPeaks matrix. A peak is not added for a sample if no signal was found in the respective data file.

Because chromatographic peaks are added to eventually previously identified peaks, it is suggested to run refineChromPeaks() with the MergeNeighboringPeaksParam() approach to merge potentially overlapping peaks.

The manualFeatures function allows to manually group identified chromatographic peaks into features by providing their index in the object's chromPeaks matrix.

Usage

```
manualChromPeaks(object, ...)

manualFeatures(object, ...)

## S4 method for signature 'MsExperiment'
manualChromPeaks(
  object,
  chromPeaks = matrix(numeric()),
```

```
  samples = seq_along(object),
  msLevel = 1L,
  chunkSize = 2L,
  BPPARAM = bpparam()
)

## S4 method for signature 'XcmsExperiment'
manualChromPeaks(
  object,
  chromPeaks = matrix(numeric()),
  samples = seq_along(object),
  msLevel = 1L,
  chunkSize = 2L,
  BPPARAM = bpparam()
)

## S4 method for signature 'XcmsExperiment'
manualFeatures(object, peakIdx = list(), msLevel = 1L)

## S4 method for signature 'OnDiskMSnExp'
manualChromPeaks(
  object,
  chromPeaks = matrix(),
  samples = seq_along(fileNames(object)),
  msLevel = 1L,
  BPPARAM = bpparam()
)

## S4 method for signature 'XCMSnExp'
manualChromPeaks(
  object,
  chromPeaks = matrix(),
  samples = seq_along(fileNames(object)),
  msLevel = 1L,
  BPPARAM = bpparam()
)

## S4 method for signature 'XCMSnExp'
manualFeatures(object, peakIdx = list(), msLevel = 1L)
```

Arguments

object	XcmsExperiment, XCMSnExp or OnDiskMSnExp object.
...	ignored.
chromPeaks	For manualChromPeaks: matrix defining the boundaries of the chromatographic peaks with one row per chromatographic peak and columns "mzmin", "mzmax", "rtmin" and "rtmax" defining the m/z and retention time region of each peak.

samples	For manualChromPeaks: optional integer defining individual samples in which the peak integration should be performed. Defaults to all samples.
msLevel	integer(1) defining the MS level in which peak integration should be performed. Only a single MS level at a time is supported. Defaults to msLevel = 1L.
chunkSize	integer(1) defining the number of files (samples) that should be loaded into memory and processed at the same time. Peak integration is then performed in parallel (per sample) on this subset data. This setting thus allows to balance between memory demand and speed (due to parallel processing). Because parallel processing can only performed on the subset of data currently loaded into memory in each iteration, the value for chunkSize should match the defined parallel setting setup. Using a parallel processing setup using 4 CPUs (separate processes) but using chunkSize = 1will not perform any parallel processing, as only the data fr to the total number of samples in an experiment will load the full MS data into memory and will thus in most settings cause an out-of-memory error.
BPPARAM	parallel processing settings (see bpparam() for details).
peakIdx	For manualFeatures: list of integer vectors with the indices of chromatographic peaks in the object's chromPeaks matrix that should be grouped into features.

Value

XcmsExperiment or XCMSnExp with the manually added chromatographic peaks or features.

Author(s)

Johannes Rainer

Examples

```
## Read a test dataset.
fls <- c(system.file("microtofq/MM14.mzML", package = "msdata"),
         system.file("microtofq/MM8.mzML", package = "msdata"))

## Define a data frame with some sample annotations
ann <- data.frame(
    injection_index = 1:2,
    sample_id = c("MM14", "MM8"))

## Import the data
library(MsExperiment)
mse <- readMsExperiment(fls)

## Define some arbitrary peak areas
pks <- cbind(
    mzmin = c(512, 234.3), mzmax = c(513, 235),
    rtmin = c(10, 33), rtmax = c(19, 50)
)
pks
```

```
res <- manualChromPeaks(mse, pks)
chromPeaks(res)

## Peaks were only found in the second file.
```

`medianFilter` *Apply a median filter to a matrix*

Description

For each element in a matix, replace it with the median of the values around it.

Usage

```
medianFilter(x, mrad, nrad)
```

Arguments

`x`	numeric matrix to median filter
`mrad`	number of rows on either side of the value to use for median calculation
`nrad`	number of rows on either side of the value to use for median calculation

Value

A matrix whose values have been median filtered

Author(s)

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

Examples

```
mat <- matrix(1:25, nrow=5)
mat
medianFilter(mat, 1, 1)
```

msn2xcmsRaw *Copy MSn data in an xcmsRaw to the MS slots*

Description

The MS2 and MSn data is stored in separate slots, and can not directly be used by e.g. findPeaks(). `msn2xcmsRaw()` will copy the MSn spectra into the "normal" `xcmsRaw` slots.

Usage

```
msn2xcmsRaw(xmsn)
```

Arguments

`xmsn`	an object of class `xcmsRaw` that contains spectra read with includeMSn=TRUE

Details

The default gap value is determined from the 90th percentile of the pair-wise differences between adjacent mass values.

Value

An xcmsRaw object

Author(s)

Steffen Neumann <sneumann@ipb-halle.de>

See Also

xcmsRaw,

Examples

```
msnfile <- system.file("microtofq/MSMSpos20_6.mzML", package = "msdata")
xrmsn <- xcmsRaw(msnfile, includeMSn=TRUE)
xr <- msn2xcmsRaw(xrmsn)
p <- findPeaks(xr, method="centWave")
```

na.flatfill *Fill in NA values at the extremes of a vector*

Description

Extend the first and last real values in a vector to fill in any NA values present.

Usage

```
na.flatfill(x)
```

Arguments

x	numeric vector with NA values

Value

Modified vector.

Author(s)

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

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	XcmsExperiment() or XCMSnExp() object 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 a test data set with detected peaks
library(MSnbase)
data(faahko_sub)
## Update the path to the files for the local system
dirname(faahko_sub) <- system.file("cdf/KO", package = "faahKO")

## Disable parallel processing for this example
register(SerialParam())

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

## Identify overlapping features
overlappingFeatures(xdata)

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

---

panel.cor *Correlation coefficient panel for pairs function*

Description

Correlation coefficient panel for pairs function.

Usage

```
panel.cor(x, y, digits = 2, prefix = "", cex.cor)
```

Arguments

`x`	first data series
`y`	second data series
`digits`	number of digits to plot
`prefix`	text to prefix the coefficients
`cex.cor`	character expansion factor

Author(s)

Colin A. Smith, <csmith@scripps.edu>, based on pairs example code

See Also

pairs

---

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,
  extendLengthMSW = FALSE,
  ...
)
```

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 *regions of interest*).
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. In detail, a first *rough* estimate of the noise is calculated and peak detection is performed only in regions in which multiple sequential signals are higher than this first estimated baseline/noise level.

`extendLengthMSW`
: `logical(1)`. If `TRUE` the "open" method of EIC extension is used, rather than the default "reflect" method.

`...`
: 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 `(maxo - baseline)/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(MsExperiment)
library(xcms)
od <- readMsExperiment(system.file("cdf/KO/ko15.CDF", package = "faahKO"))

## Extract chromatographic data for a small m/z range
mzr <- c(272.1, 272.2)
chr <- chromatogram(od, mz = mzr, rt = c(3000, 3300))[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

```
## Load the test file
faahko_sub <- loadXcmsData("faahko_sub")

## Subset to one file and drop identified chromatographic peaks
data <- dropChromPeaks(filterFile(faahko_sub, 1))

## Extract chromatographic data for a small m/z range
```

```
chr <- chromatogram(data, mz = c(272.1, 272.3), rt = c(3000, 3200))[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)
```

PercentMissingFilter *Filter features based on the percentage of missing data*

Description

The 'PercentMissingFilter' class and method enable users to filter features from an 'XcmsExperiment' or 'SummarizedExperiment' object based on the percentage (values from 1 to 100) of missing values for each features in different sample groups and filters them according to a provided threshold.

This 'filter' is part of the possible dispatch of the generic function 'filterFeatures'. Features with a percentage of missing values *higher* ('>') than the user input threshold in all sample groups will be removed (i.e. features for which the proportion of missing values is below ('<=') the threshold in at least one sample group will be retained).

Usage

```
PercentMissingFilter(threshold = 30, f = factor())

## S4 method for signature 'XcmsResult,PercentMissingFilter'
filterFeatures(object, filter, ...)

## S4 method for signature 'SummarizedExperiment,PercentMissingFilter'
filterFeatures(object, filter, assay = 1)
```

Arguments

threshold	'numeric' percentage (between 0 and 100) of accepted missing values for a feature in one sample group.
f	'vector' of the same length as the 'object', specifying the sample type for each sample in the dataset. The percentage of missing values per feature will be computed within each of these sample groups. Parameter 'f', if not already a 'factor', will be converted to one using the factor function. Samples with an 'NA' as their value in 'f' will be excluded from calculation.
object	XcmsExperiment or SummarizedExperiment. For an XcmsExperiment object, the featureValues(object) will be evaluated, and for Summarizedesxperiment the assay(object, assay). The object will be filtered.
filter	The parameter object selecting and configuring the type of filtering. It can be one of the following classes: RsdFilter, DratioFilter, PercentMissingFilter or BlankFlag.
...	Optional parameters. For object being an XcmsExperiment: parameters for the featureValues() call.
assay	For filtering of SummarizedExperiment objects only. Indicates which assay the filtering will be based on. Note that the features for the entire object will be removed, but the computations are performed on a single assay. Default is 1, which means the first assay of the object will be evaluated.

Value

For 'PercentMissingFilter': a 'PercentMissingFilter' class. 'filterFeatures' return the input object minus the features that did not met the user input threshold

Author(s)

Philippine Louail

See Also

Other Filter features in xcms: BlankFlag, DratioFilter, RsdFilter

---

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)
```

PlainTextParam *Store contents of 'MsExperiment' and 'XcmsExperiment' objects as plain text files*

Description

The 'PlainTextParam' class and method enable users to save 'MsExperiment' or 'XcmsExperiment' objects as collections of plain text files in a specified folder. Note that, while for all xcms results within the 'XcmsExperiment' can and will be exported, the full raw MS data (of the object's 'Spectra' object) will currently not be exported in plain text format. For 'Spectra' using the [MsBackendMzR()] backend, the names of the raw data files will however be exported (which enables to *restore* the full 'Spectra' respectively 'MsExperiment' objects).

For an 'MsExperiment' object, the exported files include:

- The [sampleData()] stored as a text file named *sample_data.txt*.

- The [fileNames()] of the *Spectra* object stored in a tabular format in a text file named *spectra_files.txt*.The file names will only be exported if the 'Spectra' object uses a [MsBackendMzR()] backend. For other backends no information on raw spectra data is currently exported with 'PlainTextParam'.

- Processing queue of the 'Spectra' object, ensuring that any spectra data modifications are retained. It is stored in a 'json' file named *spectra_processing_queue.json*.

For an 'XcmsExperiment' object, the exported files are the same as those for an 'MsExperiment' object, with the addition of the following:

- The [processHistory()] information of the object, stored in a 'json' file named *process_history.json*.

- The chromatographic peak information obtained with [chromPeaks()] and [chromPeaksData()], stored in tabular format in the text files *chrom_peaks.txt* and *chrom_peak_data.txt* respectively.

- The retention time information obtained with [adjustedRtime()] stored in the text file named *rtime_adjusted.txt*.

- The [featureDefinitions()] stored in a text file named *feature_definitions.txt*. Additionally, a second file named *feature_peak_index.txt* is generated to connect the features' definitions with their names.

This ‘param‘ class and method are part of the possible dispatch of the generic function ‘storeResults‘. The folder will be created by calling ‘storeResults‘. If the folder already exists, previous exports in that folder might get overwritten.

Usage

```
PlainTextParam(path = tempdir())

## S4 method for signature 'MsExperiment,PlainTextParam'
storeResults(object, param)

## S4 method for signature 'XcmsExperiment,PlainTextParam'
storeResults(object, param)
```

Arguments

path	for ‘PlainTextParam‘ ‘character(1)‘, defining where the files are going to be stored. The default will be ‘tempdir()‘.
object	MsExperiment or XcmsExperiment The data object that needs to be saved.
param	The parameter object selecting and configuring the format for saving. It can be one of the following classes: RDataParam, PlainTextParam, or MzTabMParam.

Value

for ‘PlainTextParam‘: a ‘PlainTextParam‘ class. ‘storeResults‘ does not return anything but saves the object to collections of different plain text files to a folder.

Author(s)

Philippine Louail, Johannes Rainer.

See Also

Other xcms result export formats.: RDataParam

Examples

```
## Load test data set of class `MsExperiment`
library(MsExperiment)
fls <- dir(system.file("sciex", package = "msdata"), full.names = TRUE)
pd <- data.frame(file = basename(fls),
                 sample = c("POOL_1", "POOL_2"),
                 injection_index = c(1, 19),
                group = "POOL")
rownames(pd) <- c("1", "2")
mse <- readMsExperiment(fls, sampleData = pd)

## Define param
pth = file.path(tempdir(), "test")
param <- PlainTextParam(path = pth)
```

```
## Save as a collection of plain text files
storeResults(object = mse, param = param)

## Load a test data set with detected peaks, of class `XcmsExperiment`
faahko_sub <- loadXcmsData("faahko_sub2")

## Define param
pth = file.path(tempdir(), "test")
param <- PlainTextParam(path = pth)

## Save as a collection of plain text files
storeResults(object = faahko_sub, param = param)
```

`plot.xcmsEIC` *Plot extracted ion chromatograms from multiple files*

Description

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

Arguments

`x`	the `xcmsEIC` object
`y`	optional `xcmsSet` object with peak integration data
`groupidx`	either character vector with names or integer vector with indicies of peak groups for which to plot EICs
`sampleidx`	either character vector with names or integer vector with indicies of samples for which to plot EICs
`rtrange`	a two column matrix with minimum and maximum retention times between which to return EIC data points if it has the same number of rows as the number groups in the `xcmsEIC` object, then `sampleidx` is used to subset it. otherwise, it is repeated over the length of `sampleidx` it may also be a single number specifying the time window around the peak for which to plot EIC data
`col`	color to use for plotting extracted ion chromatograms. if missing and `y` is specified, colors are taken from `unclass(sampclass(y))` and the default palette if it is the same length as the number groups in the `xcmsEIC` object, then `sampleidx` is used to subset it. otherwise, it is repeated over the length of `sampleidx`
`legtext`	text to use for legend. if `NULL` and `y` is specified, legend text is taken from the sample class information found in the `xcmsSet`
`peakint`	logical, plot integrated peak area with darkened lines (requires that `y` also be specified)
`sleep`	seconds to pause between plotting EICs
`...`	other graphical parameters

Value

A xcmsSet object.

Methods

x = "xcmsEIC" `plot.xcmsEIC(x, y, groupidx = groupnames(x), sampleidx = sampnames(x), rtrange = x@rtrange, col = rep(1, length(sampleidx)), legtext = NULL, peakint = TRUE, sleep = 0, ...)`

Author(s)

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

See Also

xcmsEIC-class, png, pdf, postscript,

---

plotAdjustedRtime *Visualization of Alignment Results*

Description

The 'plotAdjustedRtime' function plots the difference between the adjusted and *raw* retention times on the y-axis against the raw retention times on the x-axis. Each line represents the results for one sample (file). If alignment was performed using the *peak groups* method (see [adjustRtime()] for more infromation) also the peak groups used in the alignment are visualized.

Usage

```
plotAdjustedRtime(
  object,
  col = "#00000080",
  lty = 1,
  lwd = 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

object	A [XcmsExperiment()] or [XCMSnExp()] object with the alignment results.
col	color(s) for the individual lines. Has to be of length 1 or equal to the number of samples.
lty	line type for the lines of the individual samples.
lwd	line width for the lines of the individual samples.
type	plot *type* (see [par()] for options; defaults to ‘type = "l"‘).
adjustedRtime	‘logical(1)‘ whether adjusted or raw retention times should be shown on the x-axis.
xlab	the label for the x-axis.
ylab	the label for the y-axis.
peakGroupsCol	color to be used for the peak groups (only if alignment was performed using the *peak groups* method.
peakGroupsPch	point character (‘pch‘) to be used for the peak groups (only if alignment was performed using the *peak groups* method.
peakGroupsLty	line type (‘lty‘) to be used to connect points for each peak groups (only if alignment was performed using the *peak groups* method.
ylim	optional ‘numeric(2)‘ with the upper and lower limits on the y-axis.b
...	Additional arguments to be passed down to the ‘plot‘ function.

Author(s)

Johannes Rainer

Examples

```
## Load a test data set with detected peaks
faahko_sub <- loadXcmsData("faahko_sub2")

## Disable parallel processing for this example
register(SerialParam())

## Performing the peak grouping using the "peak density" method.
p <- PeakDensityParam(sampleGroups = c(1, 1, 1))
res <- groupChromPeaks(faahko_sub, 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.
plotAdjustedRtime(res, adjusted = FALSE)
grid()
```

plotChrom-methods *Plot extracted ion chromatograms from the profile matrix*

Description

Uses the pre-generated profile mode matrix to plot averaged or base peak extracted ion chromatograms over a specified mass range.

Arguments

object	the xcmsRaw object
base	logical, plot a base-peak chromatogram
ident	logical, use mouse to identify and label peaks
fitgauss	logical, fit a gaussian to the largest peak
vline	numeric vector with locations of vertical lines
...	arguments passed to profRange

Value

If ident == TRUE, an integer vector with the indecies of the points that were identified. If fitgauss == TRUE, a nls model with the fitted gaussian. Otherwise a two-column matrix with the plotted points.

Methods

object = "xcmsRaw" plotChrom(object, base = FALSE, ident = FALSE, fitgauss = FALSE, vline = numeric(0), ...)

See Also

xcmsRaw-class

plotChromatogramsOverlay *Plot multiple chromatograms into the same plot*

Description

plotOverlay draws chromatographic peak data from multiple (different) extracted ion chromatograms (EICs) into the same plot. This allows to directly compare the peak shape of these EICs in the same sample. In contrast to the plot function for MChromatograms() object, which draws the data from the same EIC across multiple samples in the same plot, this function draws the different EICs from the same sample into the same plot.

If plotChromatogramsOverlay is called on a XChromatograms object any present chromatographic peaks will also be highlighted/drawn depending on the parameters peakType, peakCol, peakBg and peakPch (see also help on the plot function for XChromatogram() object for details).

Usage

```
## S4 method for signature 'MChromatograms'
plotChromatogramsOverlay(
  object,
  col = "#00000060",
  type = "l",
  main = NULL,
  xlab = "rtime",
  ylab = "intensity",
  xlim = numeric(),
  ylim = numeric(),
  stacked = 0,
  transform = identity,
  ...
)

## S4 method for signature 'XChromatograms'
plotChromatogramsOverlay(
  object,
  col = "#00000060",
  type = "l",
  main = NULL,
  xlab = "rtime",
  ylab = "intensity",
  xlim = numeric(),
  ylim = numeric(),
  peakType = c("polygon", "point", "rectangle", "none"),
  peakBg = NULL,
  peakCol = NULL,
  peakPch = 1,
  stacked = 0,
  transform = identity,
  ...
)
```

Arguments

object	MChromatograms() or XChromatograms() object.
col	definition of the color in which the chromatograms should be drawn. Can be of length 1 or equal to nrow(object) to plot each overlayed chromatogram in a different color.
type	character(1) defing the type of the plot. By default (type = "l") each chromatogram is drawn as a line.
main	optional title of the plot. If not defined, the range of m/z values is used.
xlab	character(1) defining the x-axis label.
ylab	character(1) defining the y-axis label.
xlim	optional numeric(2) defining the x-axis limits.

ylim	optional numeric(2) defining the y-axis limits.
stacked	numeric(1) defining the part (proportion) of the y-axis to use to *stack* EICs depending on their m/z values. If stacked = 0 (the default) no stacking is performed. With stacked = 1 half of the y-axis is used for stacking and half for the intensity y-axis (i.e. the ratio between stacking and intensity y-axis is 1:1). Note that if stacking is different from 0 no y-axis and label are drawn.
transform	function to transform the intensity values before plotting. Defaults to transform = identity which plots the data as it is. With transform = log10 intensity values would be log10 transformed before plotting.
...	optional arguments to be passed to the plotting functions (see help on the base R plot function.
peakType	if object is a XChromatograms object: how chromatographic peaks should be drawn: peakType = "polygon" (the default): label the full chromatographic peak area, peakType = "rectangle": indicate the chromatographic peak by a rectangle and peakType = "point": label the chromatographic peaks' apex position with a point.
peakBg	if object is a XChromatograms object: definition of background color(s) for each chromatographic peak. Has to be either of length 1 or equal to the number of peaks in object. If not specified, the peak will be drawn in the color defined by col.
peakCol	if object is a XChromatograms object: definition of color(s) for each chromatographic peak. Has to be either of length 1 or equal to the number of peaks in object. If not specified, the peak will be drawn in the color defined by col.
peakPch	if object is a XChromatograms object: *point character* to be used to label the apex position of the chromatographic peak if peakType = "point".

Value

silently returns a list (length equal to ncol(object) of numeric (length equal to nrow(object)) with the y position of each EIC.

Author(s)

Johannes Rainer

Examples

```
## Load preprocessed data and extract EICs for some features.
library(xcms)
library(MSnbase)
xdata <- loadXcmsData()
data(xdata)
## Update the path to the files for the local system
dirname(xdata) <- c(rep(system.file("cdf", "KO", package = "faahKO"), 4),
                    rep(system.file("cdf", "WT", package = "faahKO"), 4))
## Subset to the first 3 files.
xdata <- filterFile(xdata, 1:3, keepFeatures = TRUE)
```

```
## Define features for which to extract EICs
fts <- c("FT097", "FT163", "FT165")
chrs <- featureChromatograms(xdata, features = fts)

plotChromatogramsOverlay(chrs)

## plot the overlay of EICs in the first sample
plotChromatogramsOverlay(chrs[, 1])

## Define a different color for each feature (row in chrs). By default, also
## all chromatographic peaks of a feature is labeled in the same color.
plotChromatogramsOverlay(chrs[, 1],
    col = c("#ff000040", "#00ff0040", "#0000ff40"))

## Alternatively, we can define a color for each individual chromatographic
## peak and provide this with the `peakBg` and `peakCol` parameters.
chromPeaks(chrs[, 1])

## Use a color for each of the two identified peaks in that sample
plotChromatogramsOverlay(chrs[, 1],
    col = c("#ff000040", "#00ff0040", "#0000ff40"),
    peakBg = c("#ffff0020", "#00ffff20"))

## Plotting the data in all samples.
plotChromatogramsOverlay(chrs,
    col = c("#ff000040", "#00ff0040", "#0000ff40"))

## Creating a "stacked" EIC plot: the EICs are placed along the y-axis
## relative to their m/z value. With `stacked = 1` the y-axis is split in
## half, the lower half being used for the stacking of the EICs, the upper
## half being used for the *original* intensity axis.
res <- plotChromatogramsOverlay(chrs[, 1], stacked = 1,
    col = c("#ff000040", "#00ff0040", "#0000ff40"))
## add horizontal lines for the m/z values of each EIC
abline(h = res[[1]], col = "grey", lty = 2)

## Note that this type of visualization is different than the conventional
## plot function for chromatographic data, which will draw the EICs for
## multiple samples into the same plot
plot(chrs)

## Converting the object to a MChromatograms without detected peaks
chrs <- as(chrs, "MChromatograms")

plotChromatogramsOverlay(chrs,
    col = c("#ff000040", "#00ff0040", "#0000ff40"))
```

---

plotChromPeakDensity,XCMSnExp-method

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

```
## S4 method for signature 'XCMSnExp'
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 *peak density* correspondence algorithm can be extracted. If not provided and if `object` contains feature definitions with the correspondence/ peak grouping being performed by the *peak density* method, the corresponding parameter class stored in `object` is used.
`simulate`	`logical(1)` defining whether correspondence should be simulated within the specified m/z / rt region or (with `simulate = FALSE`) whether the results from an already performed correspondence should be shown.
`col`	Color to be used for the individual samples. Length has to be 1 or equal to the number of samples in `object`.
`xlab`	`character(1)` with the label for the x-axis.
`ylab`	`character(1)` with the label for the y-axis.
`xlim`	`numeric(2)` representing the limits for the x-axis. Defaults to the range of the `rt` parameter.

main	character(1) defining the title of the plot. By default (for main = NULL) the mz-range is used.
type	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 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 mz slice of interest (e.g. containing chromatographic peaks corresponding to a known metabolite). The plot shows the individual peaks that were detected within the specified mz slice at their retention time (x-axis) and sample in which they were detected (y-axis). The density function is plotted as a black line. Parameters for the density function are taken from the param object. Grey rectangles indicate which chromatographic peaks would be grouped into a feature by the peak density correspondence method. Parameters for the algorithm are also taken from param. See groupChromPeaks() 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() for details on the *peak density* correspondence method and supported settings.

Examples

```
## Load a test data set with detected peaks
library(MSnbase)
data(faahko_sub)
## Update the path to the files for the local system
dirname(faahko_sub) <- system.file("cdf/KO", package = "faahKO")

## Plot the chromatographic peak density for a specific mz range to evaluate
## different peak density correspondence settings.
mzr <- c(305.05, 305.15)

plotChromPeakDensity(faahko_sub, mz = mzr, pch = 16,
    param = PeakDensityParam(sampleGroups = rep(1, length(fileNames(faahko_sub)))))
```

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 (x-axis) and m/z (y-axis) dimension. Each chromatographic peak is plotted as a rectangle representing its width in RT and m/z dimension.

'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,
  msLevel = 1L,
  ...
)

plotChromPeakImage(
  x,
  binSize = 30,
  xlim = NULL,
  log = FALSE,
  xlab = "retention time",
  yaxt = par("yaxt"),
  main = "Chromatographic peak counts",
  msLevel = 1L,
  ...
)
```

Arguments

x	A [XcmsExperiment()] or [XCMSnExp()] object.
file	For 'plotChromPeaks': 'integer(1)' specifying the index of the file within 'x' for which the plot should be created. Defaults to 'file = 1'.

xlim	'numeric(2)' specifying the x-axis limits (retention time dimension). Defaults to 'xlim = NULL' in which case the full retention time range of the file is used.
ylim	For 'plotChromPeaks': 'numeric(2)' specifying the y-axis limits (m/z dimension). Defaults to 'ylim = NULL' in which case the full m/z range of the file is used.
add	For 'plotChromPeaks': 'logical(1)' whether the plot should be added to an existing plot or if a new plot should be created.
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.
msLevel	'integer(1)' defining the MS level from which the peaks should be visualized.
...	Additional arguments passed to the 'plot' (for 'plotChromPeaks') and 'image' (for 'plotChromPeakImage') functions. Ignored for '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

Examples

```
## Load a test data set with detected peaks
faahko_sub <- loadXcmsData("faahko_sub2")

## plotChromPeakImage: plot an image for the identified peaks per file
plotChromPeakImage(faahko_sub)

## Show all detected chromatographic peaks from the first file
plotChromPeaks(faahko_sub)
```

```
## Plot all detected peaks from the second file and restrict the plot to a
## mz-rt slice
plotChromPeaks(faahko_sub, file = 2, xlim = c(3500, 3600), ylim = c(400, 600))
```

---

plotEIC-methods *Plot extracted ion chromatograms for specified m/z range*

Description

Plot extracted ion chromatogram for m/z values of interest. The raw data is used in contrast to plotChrom which uses data from the profile matrix.

Arguments

object	xcmsRaw object
mzrange	m/z range for EIC. Uses the full m/z range by default.
rtrange	retention time range for EIC. Uses the full retention time range by default.
scanrange	scan range for EIC
mzdec	Number of decimal places of title m/z values in the eic plot.
type	Speficies how the data should be plotted (by default as a line).
add	If the EIC should be added to an existing plot.
...	Additional parameters passed to the plotting function (e.g. col etc).

Value

A two-column matrix with the plotted points.

Methods

object = "xcmsRaw" `plotEIC(object, mzrange = numeric(), rtrange = numeric(), scanrange = numeric(), mzdec=2, type="l", add=FALSE, ...)`

Author(s)

Ralf Tautenhahn

See Also

rawEIC, xcmsRaw-class

plotFeatureGroups *Plot feature groups in the m/z-retention time space*

Description

plotFeatureGroups visualizes defined feature groups in the m/z by retention time space. Features are indicated by points with features from the same feature group being connected by a line. See featureGroups() for details on and options for feature grouping.

Usage

```
plotFeatureGroups(
  x,
  xlim = numeric(),
  ylim = numeric(),
  xlab = "retention time",
  ylab = "m/z",
  pch = 4,
  col = "#00000060",
  type = "o",
  main = "Feature groups",
  featureGroups = character(),
  ...
)
```

Arguments

x	XcmsExperiment or XCMSnExp() object with grouped features (i.e. after calling groupFeatures().
xlim	numeric(2) with the lower and upper limit for the x-axis.
ylim	numeric(2) with the lower and upper limit for the y-axis.
xlab	character(1) with the label for the x-axis.
ylab	character(1) with the label for the y-axis.
pch	the plotting character. Defaults to pch = 4 i.e. plotting features as crosses. See par() for more information.
col	color to be used to draw the features. At present only a single color is supported.
type	plotting type (see par()). Defaults to type = "o" which draws each feature as a point and connecting the features of the same feature group with a line.
main	character(1) with the title of the plot.
featureGroups	optional character of feature group IDs to draw only specified feature group(s). If not provided, all feature groups are drawn.
...	additional parameters to be passed to the lines function.

Author(s)

Johannes Rainer

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

Description

UPDATE: please use `plot()` from the `MsExperiment` or `plot(x, type = "XIC")` from the `MSnbase` package instead. See examples in the vignette for more information.

The `plotMsData` creates a plot that combines an (base peak) extracted ion chromatogram on top (rt against intensity) and a plot of rt against m/z values at the bottom.

Usage

```
plotMsData(
  x,
  main = "",
  cex = 1,
  mfrow = c(2, 1),
  grid.color = "lightgrey",
  colramp = colorRampPalette(rev(brewer.pal(9, "YlGnBu")))
)
```

Arguments

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

Author(s)

Johannes Rainer

plotPeaks-methods *Plot a grid of a large number of peaks*

Description

Plot extracted ion chromatograms for many peaks simultaneously, indicating peak integration start and end points with vertical grey lines.

Arguments

object	the xcmsRaw object
peaks	matrix with peak information as produced by findPeaks
figs	two-element vector describing the number of rows and the number of columns of peaks to plot, if missing then an approximately square grid that will fit the number of peaks supplied
width	width of chromatogram retention time to plot for each peak

Details

This function is intended to help graphically analyze the results of peak picking. It can help estimate the number of false positives and improper integration start and end points. Its output is very compact and tries to waste as little space as possible. Each plot is labeled with rounded m/z and retention time separated by a space.

Methods

object = "xcmsRaw" `plotPeaks(object, peaks, figs, width = 200)`

See Also

xcmsRaw-class, findPeaks, split.screen

plotQC *Plot m/z and RT deviations for QC purposes without external reference data*

Description

Use "democracy" to determine the average m/z and RT deviations for a grouped xcmsSet, and dependency on sample or absolute m/z

Usage

```
plotQC(object, sampNames, sampColors, sampOrder, what)
```

Arguments

object	A grouped xcmsSet
sampNames	Override sample names (e.g. with simplified names)
sampColors	Provide a set of colors (default: monochrome ?)
sampOrder	Override the order of samples, e.g. to bring them in order of measurement to detect time drift
what	A vector of which QC plots to generate. "mzdevhist": histogram of mz deviations. Should be gaussian shaped. If it is multimodal, then some peaks seem to have a systematically higher m/z deviation "rtdevhist": histogram of RT deviations. Should be gaussian shaped. If it is multimodal, then some peaks seem to have a systematically higher RT deviation "mzdevmass": Shows whether m/z deviations are absolute m/z dependent, could indicate miscalibration "mzdevtime": Shows whether m/z deviations are RT dependent, could indicate instrument drift "mzdevsample": median mz deviation for each sample, indicates outliers "rtdevsample": median RT deviation for each sample, indicates outliers

Details

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

Value

List with four matrices, each of dimension features * samples: "mz": median mz deviation for each sample "mzdev": median mz deviation for each sample "rt": median RT deviation for each sample "rtdev": median RT deviation for each sample

Author(s)

Michael Wenk, Michael Wenk <michael.wenk@student.uni-halle.de>

Examples

```
library(faahKO)
xsg <- group(faahko)

plotQC(xsg, what="mzdevhist")
plotQC(xsg, what="rtdevhist")
plotQC(xsg, what="mzdevmass")
plotQC(xsg, what="mzdevtime")
plotQC(xsg, what="mzdevsample")
plotQC(xsg, what="rtdevsample")
```

plotRaw-methods *Scatterplot of raw data points*

Description

Produce a scatterplot showing raw data point location in retention time and m/z. This plot is more useful for centroided data than continuum data.

Arguments

object	the xcmsRaw object
mzrange	numeric vector of length >= 2 whose range will be used to select the masses to plot
rtrange	numeric vector of length >= 2 whose range will be used to select the retention times to plot
scanrange	numeric vector of length >= 2 whose range will be used to select scans to plot
log	logical, log transform intensity
title	main title of the plot

Value

A matrix with the points plotted.

Methods

object = "xcmsRaw" `plotRaw(object, mzrange = numeric(), rtrange = numeric(), scanrange = numeric(), log=FALSE, title='Raw Data')`

See Also

xcmsRaw-class

plotrt-methods *Plot retention time deviation profiles*

Description

Use corrected retention times for each sample to calculate retention time deviation profiles and plot each on the same graph.

Arguments

object	the xcmsSet object
col	vector of colors for plotting each sample
ty	vector of line and point types for plotting each sample
leg	logical plot legend with sample labels
densplit	logical, also plot peak overall peak density

Methods

object = "xcmsSet" `plotrt(object, col = NULL, ty = NULL, leg = TRUE, densplit = FALSE)`

See Also

xcmsSet-class, retcor

---

plotScan-methods *Plot a single mass scan*

Description

Plot a single mass scan using the impulse representation. Most useful for centroided data.

Arguments

object	the xcmsRaw object
scan	integer with number of scan to plot
mzrange	numeric vector of length >= 2 whose range will be used to select masses to plot
ident	logical, use mouse to interactively identify and label individual masses

Methods

object = "xcmsRaw" `plotScan(object, scan, mzrange = numeric(), ident = FALSE)`

See Also

xcmsRaw-class

plotSpec-methods *Plot mass spectra from the profile matrix*

Description

Uses the pre-generated profile mode matrix to plot mass spectra over a specified retention time range.

Arguments

object	the xcmsRaw object
ident	logical, use mouse to identify and label peaks
vline	numeric vector with locations of vertical lines
...	arguments passed to profRange

Value

If ident == TRUE, an integer vector with the indecies of the points that were identified. Otherwise a two-column matrix with the plotted points.

Methods

object = "xcmsRaw" `plotSpec(object, ident = FALSE, vline = numeric(0), ...)`

See Also

xcmsRaw-class

plotSurf-methods *Plot profile matrix 3D surface using OpenGL*

Description

This method uses the rgl package to create interactive three dimensonal representations of the profile matrix. It uses the terrain color scheme.

Arguments

object	the xcmsRaw object
log	logical, log transform intensity
aspect	numeric vector with aspect ratio of the m/z, retention time and intensity components of the plot
...	arguments passed to profRange

Details

The rgl package is still in development and imposes some limitations on the output format. A bug in the axis label code means that the axis labels only go from 0 to the aspect ratio constant of that axis. Additionally the axes are not labeled with what they are.

It is important to only plot a small portion of the profile matrix. Large portions can quickly overwhelm your CPU and memory.

Methods

object = "xcmsRaw" `plotSurf(object, log = FALSE, aspect = c(1, 1, .5), ...)`

See Also

xcmsRaw-class

---

plotTIC-methods *Plot total ion count*

Description

Plot chromatogram of total ion count. Optionally allow identification of target peaks and viewing/identification of individual spectra.

Arguments

`object`	the `xcmsRaw` object
`ident`	logical, use mouse to identify and label chromatographic peaks
`msident`	logical, use mouse to identify and label spectral peaks

Value

If `ident == TRUE`, an integer vector with the indecies of the points that were identified. Otherwise a two-column matrix with the plotted points.

Methods

object = "xcmsRaw" `plotTIC(object, ident = FALSE, msident = FALSE)`

See Also

xcmsRaw-class

`ProcessHistory-class` *Tracking data processing*

Description

Objects of the type `ProcessHistory` allow to keep track of any data processing step in an metabolomics experiment. They are created by the data processing methods, such as `findChromPeaks` and added to the corresponding results objects. Thus, usually, users don't need to create them.

The `XProcessHistory` extends the `ProcessHistory` by adding a slot `param` that allows to store the actual parameter class of the processing step.

`processParam`, `processParam<-`: get or set the parameter class from an `XProcessHistory` object.

`msLevel`: returns the MS level on which a certain analysis has been performed, or `NA` if not defined.

The `processType` method returns a character specifying the processing step *type*.

The `processDate` extracts the start date of the processing step.

The `processInfo` extracts optional additional information on the processing step.

The `fileIndex` extracts the indices of the files on which the processing step was applied.

Usage

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

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

## S4 method for signature 'XProcessHistory'
processParam(object)

## S4 method for signature 'XProcessHistory'
msLevel(object)

## S4 method for signature 'ProcessHistory'
processType(object)

## S4 method for signature 'ProcessHistory'
processDate(object)

## S4 method for signature 'ProcessHistory'
processInfo(object)

## S4 method for signature 'ProcessHistory'
fileIndex(object)
```

Arguments

`object`	A `ProcessHistory` or `XProcessHistory` object.

Value

For `processParam`: a parameter object extending the `Param` class.

The `processType` method returns a character string with the processing step type.

The `processDate` method returns a character string with the time stamp of the processing step start.

The `processInfo` method returns a character string with optional additional informations.

The `fileIndex` method returns a integer vector with the index of the files/samples on which the processing step was applied.

Slots

`type` character(1): string defining the type of the processing step. This string has to match predefined values. Use `processHistoryTypes` to list them.

`date` character(1): date time stamp when the processing step was started.

`info` character(1): optional additional information.

`fileIndex` integer of length 1 or > 1 to specify on which samples of the object the processing was performed.

`error` (ANY): used to store eventual calculation errors.

`param` (Param): an object of type `Param` (e.g. `CentWaveParam`) specifying the settings of the processing step.

`msLevel: integer` definining the MS level(s) on which the analysis was performed.

Author(s)

Johannes Rainer

`profGenerate` *Generation of profile data*

Description

Generates profile (binned) data in a given range from an indexed pair of vectors.

Usage

```
profBin(x, y, num, xstart = min(x), xend = max(x), param = list())
profBinM(x, y, zidx, num, xstart = min(x), xend = max(x), NAOK = FALSE,
         param = list())
profBinLin(x, y, num, xstart = min(x), xend = max(x), param = list())
profBinLinM(x, y, zidx, num, xstart = min(x), xend = max(x), NAOK = FALSE,
            param = list())
profBinLinBase(x, y, num, xstart = min(x), xend = max(x), param = list())
profBinLinBaseM(x, y, zidx, num, xstart = min(x), xend = max(x), NAOK = FALSE,
                param = list())
profIntLin(x, y, num, xstart = min(x), xend = max(x), param = list())
```

```
profIntLinM(x, y, zidx, num, xstart = min(x), xend = max(x), NAOK = FALSE,
            param = list())
profMaxIdx(x, y, num, xstart = min(x), xend = max(x), param = list())
profMaxIdxM(x, y, zidx, num, xstart = min(x), xend = max(x), NAOK = FALSE,
            param = list())
```

Arguments

x	numeric vector of value positions
y	numeric vector of values to bin
zidx	starting position of each new segment
num	number of equally spaced x bins
xstart	starting x value
xend	ending x value
NAOK	allow NA values (faster)
param	parameters for profile generation

Details

These functions take a vector of unequally spaced y values and transform them into either a vector or matrix, depending on whether there is an index or not. Each point in the vector or matrix represents the data for the point centered at its corresponding x value, plus or minus half the x step size (xend-xstart/(num-1)).

The Bin functions set each matrix or vector value to the maximal point that gets binned into it.

The BinLin functions do the same except that they linearly interpolate values into which nothing was binned.

The BinLinBase functions do the same except that they populate empty parts of spectra with a base value. They take to two parameters: 1) baselevel, the intensity level to fill in for empty parts of the spectra. It defaluts to half of the minimum intensity. 2) basespace, the m/z length after which the signal will drop to the base level. Linear interpolation will be used between consecuitive data points falling within 2*basespace of eachother. It defaluts to 0.075.

The IntLin functions set each matrix or vector value to the integral of the linearly interpolated data from plus to minus half the step size.

The MaxIdx functions work similarly to the Bin functions execpt that the return the integer index of which x,y pair would be placed in a particular cell.

Value

For prof*, a numeric vector of length num.

For prof*M, a matrix with dimensions num by length(zidx).

For MaxIdx, the data type is integer, for all others it is double.

Note

There are some issues with the profBinLin method, see https://github.com/sneumann/xcms/issues/46 and https://github.com/sneumann/xcms/issues/49. Thus it is suggested to use the functions binYonX in combination with imputeLinInterpol instead.

Author(s)

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

Examples

```
## Not run:
    library(faahKO)
    cdfpath <- system.file("cdf", package = "faahKO")
    cdffiles <- list.files(cdfpath, recursive = TRUE, full.names = TRUE)
    xraw <- xcmsRaw(cdffiles[1])

    image(xraw) ## not how with intLin the intensity's blur
    profMethod(xraw) <- "bin"
    image(xraw) ## now with 'bin' there is no blurring good for centroid data
    ##try binlinbase for profile data

## End(Not run)
```

---

profMat,MsExperiment-method

The profile matrix

Description

The *profile* matrix is an n x m matrix, n (rows) representing equally spaced m/z values (bins) and m (columns) the retention time of the corresponding scans. Each cell contains the maximum intensity measured for the specific scan and m/z values falling within the m/z bin.

```
The `profMat` method creates a new profile matrix or returns the
profile matrix within the object's `@env` slot, if available.
Settings for the profile matrix generation, such as `step` (the bin
size), `method` or additional settings are extracted from the
respective slots of the `xcmsRaw` object.
Alternatively it is possible to specify all of the settings as
additional parameters.

For [MsExperiment()] or [XcmsExperiment()] objects, the method returns
a `list` of profile matrices, one for each sample in `object`. Using
parameter `fileIndex` it is also possible to create a profile matrix only
for selected samples (files).
```

Usage

```
## S4 method for signature 'MsExperiment'
profMat(
  object,
  method = "bin",
  step = 0.1,
  baselevel = NULL,
  basespace = NULL,
  mzrange. = NULL,
  fileIndex = seq_along(object),
  chunkSize = 1L,
  msLevel = 1L,
  BPPARAM = bpparam(),
  ...
)

## S4 method for signature 'xcmsRaw'
profMat(object, method, step, baselevel, basespace, mzrange.)
```

Arguments

object	An xcmsRaw, OnDiskMSnExp, XCMSnExp, MsExperiment or XcmsExperiment object.
method	character(1) defining 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 binnind. If not provided, the whole m/z value range is used.
fileIndex	For MsExperiment or XcmsExperiment: integer defining the idex (or indices) of the sample(s) from which the profile matrix should be created.
chunkSize	For MsExperiment or XcmsExperiment: integer(1) defining the number of files from which data should be loaded and processed in one iteration. By default one file at a time is processed chunkSize = 1L which requires less memory. For parallel processing, the chunkSize should be >= than the number of parallel processes that should be used.

msLevel	For MsExperiment or XcmsExperiment: integer(1) defining the MS level from which the profile matrix should be generated.
BPPARAM	For MsExperiment or XcmsExperiment: parallel processing setup. See bpparam() for more details. Defaults to BPPARAM = bpparam().
...	ignored.

Details

Profile matrix generation methods:

- "bin": The default profile matrix generation method that does a simple binning, i.e. aggregating of intensity values falling within an m/z bin.
- "binlin": Binning followed by linear interpolation to impute missing values. The value for m/z bins without a measured intensity are inferred by a linear interpolation between neighboring bins with a measured intensity.
- "binlinbase": Binning followed by a linear interpolation to impute values for empty elements (m/z bins) within a user-definable proximity to non-empty elements while stetting the element's value to the baselevel otherwise. See impute = "linbase" parameter of imputeLinInterpol() for more details.
- "intlin": Set the elements' values to the integral of the linearly interpolated data from plus to minus half the step size.

Value

profMat returns the profile matrix (rows representing scans, columns equally spaced m/z values). For object being a MsExperiment or XcmsExperiment, the method returns a list of profile matrices, one for each file (sample).

Author(s)

Johannes Rainer

Examples

```
file <- system.file('cdf/KO/ko15.CDF', package = "faahKO")
## Load the data without generating the profile matrix (profstep = 0)
xraw <- xcmsRaw(file, profstep = 0)
## Extract the profile matrix
profmat <- profMat(xraw, step = 0.3)
dim(profmat)
## If not otherwise specified, the settings from the xraw object are used:
profinfo(xraw)
## To extract a profile matrix with linear interpolation use
profmat <- profMat(xraw, step = 0.3, method = "binlin")
## Alternatively, the profMethod of the xraw objects could be changed
profMethod(xraw) <- "binlin"
profmat_2 <- profMat(xraw, step = 0.3)
all.equal(profmat, profmat_2)
```

profMedFilt-methods *Median filtering of the profile matrix*

Description

Apply a median filter of given size to a profile matrix.

Arguments

object	the xcmsRaw object
massrad	number of m/z grid points on either side to use for median calculation
scanrad	number of scan grid points on either side to use for median calculation

Methods

object = "xcmsRaw" `profMedFilt(object, massrad = 0, scanrad = 0)`

See Also

xcmsRaw-class, medianFilter

profMethod-methods *Get and set method for generating profile data*

Description

These methods get and set the method for generating profile (matrix) data from raw mass spectral data. It can currently be bin, binlin, binlinbase, or intlin.

Methods

object = "xcmsRaw" `profMethod(object)`

See Also

xcmsRaw-class, profMethod, profBin, plotSpec, plotChrom, findPeaks

profRange-methods *Specify a subset of profile mode data*

Description

Specify a subset of the profile mode matrix given a mass, time, or scan range. Allow flexible user entry for other functions.

Arguments

object	the xcmsRaw object
mzrange	single numeric mass or vector of masses
rtrange	single numeric time (in seconds) or vector of times
scanrange	single integer scan index or vector of indecies
...	arguments to other functions

Details

This function handles selection of mass/time subsets of the profile matrix for other functions. It allows the user to specify such subsets in a variety of flexible ways with minimal typing.

Because R does partial argument matching, mzrange, scanrange, and rtrange can be specified in short form using m=, s=, and t=, respectively. If both a scanrange and rtrange are specified, then the rtrange specification takes precedence.

When specifying ranges, you may either enter a single number or a numeric vector. If a single number is entered, then the closest single scan or mass value is selected. If a vector is entered, then the range is set to the range() of the values entered. That allows specification of ranges using shortened, slightly non-standard syntax. For example, one could specify 400 to 500 seconds using any of the following: t=c(400,500), t=c(500,400), or t=400:500. Use of the sequence operator (:) can save several keystrokes when specifying ranges. However, while the sequence operator works well for specifying integer ranges, fractional ranges do not always work as well.

Value

A list with the folloing items:

mzrange	numeric vector with start and end mass
masslab	textual label of mass range
massidx	integer vector of mass indecies
scanrange	integer vector with stat ane end scans
scanlab	textual label of scan range
scanidx	integer vector of scan range
rtrange	numeric vector of start and end times
timelab	textual label of time range

Methods

object = "xcmsRaw" `profRange(object, mzrange = numeric(), rtrange = numeric(), scanrange = numeric(), ...)`

See Also

xcmsRaw-class

`profStep-methods` *Get and set m/z step for generating profile data*

Description

These methods get and set the m/z step for generating profile (matrix) data from raw mass spectral data. Smaller steps yield more precision at the cost of greater memory usage.

Methods

object = "xcmsRaw" `profStep(object)`

See Also

xcmsRaw-class, profMethod

Examples

```
## Not run:
library(faahKO)
cdfpath <- system.file("cdf", package = "faahKO")
cdffiles <- list.files(cdfpath, recursive = TRUE, full.names = TRUE)
xset <- xcmsRaw(cdffiles[1])

xset
plotSurf(xset, mass=c(200,500))

profStep(xset)<-0.1 ## decrease the bin size to get better resolution
plotSurf(xset, mass=c(200, 500))
##works nicer on high resolution data.

## End(Not run)
```

pval *Generate p-values for a vector of t-statistics*

Description

Generate p-values for a vector of Welch's two-sample t-statistics based on the t distribution.

Usage

```
pval(X, classlabel, teststat)
```

Arguments

X	original data matrix
classlabel	integer vector with classlabel
teststat	numeric vector with Welch's two-sample t-statistics

Value

A numeric vector of p-values.

Author(s)

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

quantify,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. Parameter 'msLevel' allows to choose a specific MS level for which feature values should be returned (given that features have been defined for that MS level).

`quantify,XCMSnExp`: return the preprocessing results as an `SummarizedExperiment` object containing the feature abundances as assay matrix, the feature definitions (returned by `featureDefinitions`) as `rowData` and the phenotype information as `colData`. This is an ideal container for further processing of the data. Internally, the `featureValues` method is used to extract the feature abundances, parameters for that method can be passed to `quantify` with `...`.

Usage

```
## S4 method for signature 'XCMSnExp'
quantify(object, ...)

## S4 method for signature 'XCMSnExp'
featureValues(
  object,
  method = c("medret", "maxint", "sum"),
  value = "into",
  intensity = "into",
  filled = TRUE,
  missing = NA,
  msLevel = integer()
)
```

Arguments

object	A XCMSnExp object providing the feature definitions.
...	For quantify: additional parameters to be passed on to the featureValues method.
method	character specifying the method to resolve multi-peak mappings within the same sample, i.e. to define the *representative* peak for a feature in samples where more than one peak was assigned to the feature. If "medret": select the peak closest to the median retention time of the feature. If "maxint": select the peak yielding the largest signal. If "sum": sum the values (only if value is "into" or "maxo".
value	character specifying the name of the column in chromPeaks(object) that should be returned. Defaults to "into" in which case the integrated peak area is returned. To get the index of the peak in the chromPeaks(object) matrix use "index".
intensity	character specifying the name of the column in the chromPeaks(objects) matrix containing the intensity value of the peak that should be used for the conflict resolution if method = "maxint".
filled	logical(1) specifying whether values for filled-in peaks should be returned or not. If filled = FALSE, an NA is returned in the matrix for the respective peak. See fillChromPeaks for details on peak filling.
missing	how missing values should be reported. Allowed values are NA (the default), a numeric or missing = "rowmin_half". The latter replaces any NA with half of the row's minimal (non-missing) value.
msLevel	for 'featureValues': 'integer' defining the MS level(s) for which feature values should be returned. By default, values for features defined for all MS levels are returned.

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).

For quantify: a SummarizedExperiment representing the preprocessing results.

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.

featureChromatograms to extract ion chromatograms for each feature.

hasFeatures to evaluate whether the XCMSnExp provides feature definitions.

groupval for the equivalent method on xcmsSet objects.

---

rawEIC-methods *Get extracted ion chromatograms for specified m/z range*

Description

Generate extracted ion chromatogram for m/z values of interest. The raw data is used in contrast to getEIC which uses data from the profile matrix (i.e. values binned along the M/Z dimension).

Arguments

object	xcmsRaw object
mzrange	m/z range for EIC
rtrange	retention time range for EIC
scanrange	scan range for EIC

Value

A list of :

scan	scan number
intensity	added intensity values

Methods

object = "xcmsRaw" `rawEIC(object, mzrange = numeric(), rtrange = numeric(), scanrange = numeric())`

Author(s)

Ralf Tautenhahn

See Also

`xcmsRaw-class`

`rawMat-methods` *Get a raw data matrix*

Description

Returns a matrix with columns for time, m/z, and intensity that represents the raw data from a chromatography mass spectrometry experiment.

Arguments

`object`	The container of the raw data
`mzrange`	Subset by m/z range
`rtrange`	Subset by retention time range
`scanrange`	Subset by scan index range
`log`	Whether to log transform the intensities

Value

A numeric matrix with three columns: time, mz and intensity.

Methods

object = "xcmsRaw" `rawMat(object, mzrange = numeric(), rtrange = numeric(), scanrange = numeric(), log=FALSE)`

Author(s)

Michael Lawrence

See Also

`plotRaw` for plotting the raw intensities

RDataParam *Store 'XcmsExperiment' object as .RData file*

Description

The 'RDataParam' class and method allow users to save an 'XcmsExperiment' object as an .RData file with a chosen filename. The object gets exported using ['save()'] function. This 'param' class and method are part of the possible dispatch of the generic function 'storeResults'.

Usage

```
RDataParam(fileName = tempfile())

## S4 method for signature 'XcmsExperiment,RDataParam'
storeResults(object, param)
```

Arguments

fileName	for 'RDataParam' 'character(1)', defining the file name. The default will be 'tempfile()'.
object	MsExperiment or XcmsExperiment The data object that needs to be saved.
param	The parameter object selecting and configuring the format for saving. It can be one of the following classes: RDataParam, PlainTextParam, or MzTabMParam.

Value

for 'RDataParam': a 'RDataParam' class. 'storeResults' does not return anything but saves the object to a RData file.

Author(s)

Philippine Louail

See Also

Other xcms result export formats.: PlainTextParam

Examples

```
## Load a test data set with detected peaks
faahko_sub <- loadXcmsData("faahko_sub2")

## Define param
param <- RDataParam(fileName = "example_xcms_object")

## Save as RData
storeResults(object = faahko_sub, param = param)
```

reconstructChromPeakSpectra *Data independent acquisition (DIA): reconstruct MS2 spectra*

Description

Reconstructs MS2 spectra for each MS1 chromatographic peak (if possible) for data independent acquisition (DIA) data (such as SWATH). See the *LC-MS/MS analysis* vignette for more details and examples.

Usage

```
reconstructChromPeakSpectra(object, ...)

## S4 method for signature 'XcmsExperiment'
reconstructChromPeakSpectra(
  object,
  expandRt = 0,
  diffRt = 2,
  minCor = 0.8,
  intensity = "maxo",
  peakId = rownames(chromPeaks(object, msLevel = 1L)),
  BPPARAM = bpparam()
)

## S4 method for signature 'XCMSnExp'
reconstructChromPeakSpectra(
  object,
  expandRt = 0,
  diffRt = 2,
  minCor = 0.8,
  intensity = "maxo",
  peakId = rownames(chromPeaks(object, msLevel = 1L)),
  BPPARAM = bpparam(),
  return.type = c("Spectra", "MSpectra")
)
```

Arguments

object	XCMSnExp with identified chromatographic peaks.
...	ignored.
expandRt	numeric(1) allowing to expand the retention time range for extracted ion chromatograms by a constant value (for the peak shape correlation). Defaults to expandRt = 0 hence correlates only the signal included in the identified chromatographic peaks.

diffRt	numeric(1) defining the maximal allowed difference between the retention time of the chromatographic peak (apex) and the retention times of MS2 chromatographic peaks (apex) to consider them as representing candidate fragments of the original ion.
minCor	numeric(1) defining the minimal required correlation coefficient for MS2 chromatographic peaks to be considered for MS2 spectrum reconstruction.
intensity	character(1) defining the column in the chromPeaks matrix that should be used for the intensities of the reconstructed spectra's peaks. The same value from the MS1 chromatographic peaks will be used as precursorIntensity of the resulting spectra.
peakId	optional character vector with peak IDs (i.e. rownames of chromPeaks) of MS1 peaks for which MS2 spectra should be reconstructed. By default they are reconstructed for all MS1 chromatographic peaks.
BPPARAM	parallel processing setup. See bpparam() for more information.
return.type	character(1) defining the type of the returned object. Only return.type = "Spectra" is supported, return.type = "MSpectra" is deprecated.

Details

In detail, the function performs for each MS1 chromatographic peak:

- Identify all MS2 chromatographic peaks from the isolation window containing the m/z of the ion (i.e. the MS1 chromatographic peak) with approximately the same retention time than the MS1 peak (accepted rt shift can be specified with the diffRt parameter).
- Correlate the peak shapes of the candidate MS2 chromatographic peaks with the peak shape of the MS1 peak retaining only MS2 chromatographic peaks for which the correlation is > minCor.
- Reconstruct the MS2 spectrum using the m/z of all above selected MS2 chromatographic peaks and their intensity (either "maxo" or "into"). Each MS2 chromatographic peak selected for an MS1 peak will thus represent one **mass peak** in the reconstructed spectrum.

The resulting Spectra() object provides also the peak IDs of the MS2 chromatographic peaks for each spectrum as well as their correlation value with spectra variables *ms2_peak_id* and *ms2_peak_cor*.

Value

- Spectra() object (defined in the Spectra package) with the reconstructed MS2 spectra for all MS1 peaks in object. Contains empty spectra (i.e. without m/z and intensity values) for MS1 peaks for which reconstruction was not possible (either no MS2 signal was recorded or the correlation of the MS2 chromatographic peaks with the MS1 chromatographic peak was below threshold minCor. Spectra variables "ms2_peak_id" and "ms2_peak_cor" (of type CharacterList() and NumericList() with length equal to the number of peaks per reconstructed MS2 spectrum) providing the IDs and the correlation of the MS2 chromatographic peaks from which the MS2 spectrum was reconstructed. As retention time the median retention times of all MS2 chromatographic peaks used for the spectrum reconstruction is reported. The MS1 chromatographic peak intensity is reported as the reconstructed spectrum's precursorIntensity value (see parameter intensity above).

Author(s)

Johannes Rainer, Michael Witting

See Also

`findChromPeaksIsolationWindow()` for the function to perform MS2 peak detection in DIA isolation windows and for examples.

---

rectUnique *Determine a subset of rectangles with unique, non-overlapping areas*

Description

Given a matrix of rectangular areas, this function determines a subset of those rectangles that do not overlap. Rectangles are preserved on a first come, first served basis, with user control over the order in which the rectangles are processed.

Usage

```
rectUnique(m, order = seq(length = nrow(m)), xdiff = 0, ydiff = 0)
```

Arguments

`m`	four column matrix defining rectangular areas
`order`	order in which matrix columns should be scanned
`xdiff`	maximum space between overlapping rectangles in x dimension
`ydiff`	maximum space between overlapping rectangles in y dimension

Details

The `m` matrix must contain four colums defining the position of rectangle sides in the folloing order: left, right, bottom, top. This function is currently implemented in `C` using a an algorithm with quadratic running time.

Value

A logical vector indicating which rows should be kept.

Author(s)

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

Examples

```
m <- rbind(c(0,4,0,3), c(1,3,2,6), c(3,6,4,6))
plot(0, 0, type = "n", xlim=range(m[,1:2]), ylim=range(m[,3:4]))
rect(m[,1], m[,3], m[,2], m[,4])
xcms:::rectUnique(m)
# Changing order of processing
xcms:::rectUnique(m, c(2,1,3))
# Requiring border spacing
xcms:::rectUnique(m, ydiff = 1)
# Allowing adjacent boxes
xcms:::rectUnique(m, c(2,1,3), xdiff = -0.00001)
# Allowing interpenetration
xcms:::rectUnique(m, xdiff = -1.00001, ydiff = -1.00001)
```

---

refineChromPeaks *Refine Identified Chromatographic Peaks*

Description

The `refineChromPeaks` method performs a post-processing of the chromatographic peak detection step to eventually clean and improve the results. The function can be applied to a `XcmsExperiment()` or `XCMSnExp()` object **after** peak detection with `findChromPeaks()`. The type of peak refinement and cleaning can be defined, along with all its settings, using one of the following parameter objects:

- `CleanPeaksParam`: remove chromatographic peaks with a retention time range larger than the provided maximal acceptable width (`maxPeakwidth`).
- `FilterIntensityParam`: remove chromatographic peaks with intensities below the specified threshold. By default (with `nValues = 1`) values in the `chromPeaks` matrix are evaluated: all peaks with a value in the column defined with parameter `value` that are `>=` a threshold (defined with parameter `threshold`) are retained. If `nValues` is larger than 1, the individual peak intensities from the raw MS files are evaluated: chromatographic peaks with at least `nValues` mass peaks `>= threshold` are retained.
- `MergeNeighboringPeaksParam`: peak detection sometimes fails to identify a chromatographic peak correctly, especially for broad peaks and if the peak shape is irregular (mostly for HILIC data). In such cases several smaller peaks are reported. Also, peak detection with *centWave* can result in partially or completely overlapping peaks. This method aims to reduce such peak detection artifacts by merging chromatographic peaks that are overlapping or close in RT and m/z dimension (considering also the measured signal between them). See section *Details for MergeNeighboringPeaksParam* for details and a comprehensive description of the approach.

`refineChromPeaks` methods will always remove feature definitions, because a call to this method can change or remove identified chromatographic peaks, which may be part of features.

Usage

```
refineChromPeaks(object, param, ...)
```

```
## S4 method for signature 'XcmsExperiment,CleanPeaksParam'
refineChromPeaks(object, param = CleanPeaksParam(), msLevel = 1L)

## S4 method for signature 'XcmsExperiment,MergeNeighboringPeaksParam'
refineChromPeaks(
  object,
  param,
  msLevel = 1L,
  chunkSize = 2L,
  BPPARAM = bpparam()
)

## S4 method for signature 'XcmsExperiment,FilterIntensityParam'
refineChromPeaks(
  object,
  param,
  msLevel = 1L,
  chunkSize = 2L,
  BPPARAM = bpparam()
)

CleanPeaksParam(maxPeakwidth = 10)

MergeNeighboringPeaksParam(
  expandRt = 2,
  expandMz = 0,
  ppm = 10,
  minProp = 0.75
)

FilterIntensityParam(threshold = 0, nValues = 1L, value = "maxo")

## S4 method for signature 'XCMSnExp,CleanPeaksParam'
refineChromPeaks(object, param = CleanPeaksParam(), msLevel = 1L)

## S4 method for signature 'XCMSnExp,MergeNeighboringPeaksParam'
refineChromPeaks(
  object,
  param = MergeNeighboringPeaksParam(),
  msLevel = 1L,
  BPPARAM = bpparam()
)

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

```
  BPPARAM = bpparam()
)
```

Arguments

object	XCMSnExp or XcmsExperiment object with identified chromatographic peaks.
param	Object defining the refinement method and its settings.
...	ignored.
msLevel	integer defining for which MS level(s) the chromatographic peaks should be cleaned.
chunkSize	For refineChromPeaks if object is either an XcmsExperiment: integer(1) defining the number of files (samples) that should be loaded into memory and processed at the same time. Peak refinement is then performed in parallel (per sample) on this subset data. This setting thus allows to balance between memory demand and speed (due to parallel processing). Because parallel processing can only performed on the subset of data currently loaded into memory in each iteration, the value for chunkSize should match the defined parallel setting setup. Using a parallel processing setup using 4 CPUs (separate processes) but using chunkSize = 1will not perform any parallel processing, as only the data from one sample i to the total number of samples in an experiment will load the full MS data into memory and will thus in most settings cause an out-of-memory error.
BPPARAM	parameter object to set up parallel processing. Uses the default parallel processing setup returned by bpparam(). See bpparam() for details and examples.
maxPeakwidth	For CleanPeaksParam: numeric(1) defining the maximal allowed peak width (in retention time).
expandRt	For MergeNeighboringPeaksParam: numeric(1) defining by how many seconds the retention time window is expanded on both sides to check for overlapping peaks.
expandMz	For MergeNeighboringPeaksParam: numeric(1) constant value by which the m/z range of each chromatographic peak is expanded (on both sides!) to check for overlapping peaks.
ppm	For MergeNeighboringPeaksParam: numeric(1) defining a m/z relative value (in parts per million) by which the m/z range of each chromatographic peak is expanded (on each side) to check for overlapping peaks.
minProp	For MergeNeighboringPeaksParam: numeric(1) between 0 and 1 representing the proporion of intensity required for peaks to be joined. See description for more details. With default (minProp = 0.75) only peaks are joined if the signal half way between them is larger than 75% of the smallest of the two peak's "maxo" (maximal intensity at peak apex).
threshold	For FilterIntensityParam: numeric(1) defining the threshold below which peaks are removed.
nValues	For FilterIntensityParam: integer(1) defining the number of data points (for each chromatographic peak) that have to be >= threshold. Defaults to nValues = 1.
value	For FilterIntensityParam: character(1) defining the name of the column in chromPeaks that contains the values to be used for the filtering.

Value

XCMSnExp or XcmsExperiment object with the refined chomatographic peaks.

Details for MergeNeighboringPeaksParam

For peak refinement using the MergeNeighboringPeaksParam, chromatographic peaks are first expanded in m/z and retention time dimension (based on parameters expandMz, ppm and expandRt) and subsequently grouped into sets of merge candidates if they are (after expansion) overlapping in both m/z and rt (within the **same** sample). Note that **each** peak gets expanded by expandRt and expandMz, thus peaks differing by less than 2 * expandMz (or 2 * expandRt) will be evaluated for merging. Peak merging is performed along the retention time axis, i.e., the peaks are first ordered by their "rtmin" and merge candidates are defined iteratively starting with the first peak. Candidate peaks are merged if the average intensity of the 3 data points in the middle position between them (i.e., at half the distance between "rtmax" of the first and "rtmin" of the second peak) is larger than a certain proportion (minProp) of the smaller ("maxo") intensity of both peaks. In cases in which this calculated mid point is not located between the apexes of the two peaks (e.g., if the peaks are largely overlapping) the average signal intensity at half way between the apexes is used instead. Candidate peaks are not merged if all 3 data points between them have NA intensities.

Merged peaks get the "mz", "rt", "sn" and "maxo" values from the peak with the largest signal ("maxo") as well as its row in the metadata of the peak (chromPeakData). The "rtmin" and "rtmax" of the merged peaks are updated and "into" is recalculated based on all signal between "rtmin" and "rtmax" and the newly defined "mzmin" and "mzmax" (which is the range of "mzmin" and "mzmax" of the merged peaks after expanding by expandMz and ppm). The reported "mzmin" and "mzmax" for the merged peak represents the m/z range of all non-NA intensities used for the calculation of the peak signal ("into").

Author(s)

Johannes Rainer, Mar Garcia-Aloy

Examples

```
## Load a test data set with detected peaks
library(xcms)
library(MsExperiment)
faahko_sub <- loadXcmsData("faahko_sub2")

## Disable parallel processing for this example
register(SerialParam())

####
## CleanPeaksParam:

## Distribution of chromatographic peak widths
quantile(chromPeaks(faahko_sub)[, "rtmax"] - chromPeaks(faahko_sub)[, "rtmin"])

## Remove all chromatographic peaks with a width larger 60 seconds
data <- refineChromPeaks(faahko_sub, param = CleanPeaksParam(60))

quantile(chromPeaks(data)[, "rtmax"] - chromPeaks(data)[, "rtmin"])
```

```
####
## FilterIntensityParam:

## Remove all peaks with a maximal intensity below 50000
res <- refineChromPeaks(faahko_sub,
    param = FilterIntensityParam(threshold = 50000))

nrow(chromPeaks(faahko_sub))
nrow(chromPeaks(res))

####
## MergeNeighboringPeaksParam:

## Subset to a single file
xd <- filterFile(faahko_sub, file = 1)

## Example of a split peak that will be merged
mzr <- 305.1 + c(-0.01, 0.01)
chr <- chromatogram(xd, mz = mzr, rt = c(2700, 3700))
plot(chr)

## Combine the peaks
res <- refineChromPeaks(xd, param = MergeNeighboringPeaksParam(expandRt = 4))
chr_res <- chromatogram(res, mz = mzr, rt = c(2700, 3700))
plot(chr_res)

## Example of a peak that was not merged, because the signal between them
## is lower than the cut-off minProp
mzr <- 496.2 + c(-0.01, 0.01)
chr <- chromatogram(xd, mz = mzr, rt = c(3200, 3500))
plot(chr)
chr_res <- chromatogram(res, mz = mzr, rt = c(3200, 3500))
plot(chr_res)
```

`removeIntensity,Chromatogram-method`

Remove intensities from chromatographic data

Description

`removeIntensities` allows to remove intensities from chromatographic data matching certain conditions (depending on parameter `which`). The intensities are actually not *removed* but replaced with `NA_real_`. To actually **remove** the intensities (and the associated retention times) use `clean()` afterwards.

Parameter `which` allows to specify which intensities should be replaced by `NA_real_`. By default (`which = "below_threshod"` intensities below `threshold` are removed. If `x` is a `XChromatogram` or `XChromatograms` object (and hence provides also chromatographic peak definitions within the object) `which = "outside_chromPeak"` can be selected which removes any intensity which is outside the boundaries of identified chromatographic peak(s) in the chromatographic data.

Note that `filterIntensity()` might be a better approach to subset/filter chromatographic data.

Usage

```
## S4 method for signature 'Chromatogram'
removeIntensity(object, which = "below_threshold", threshold = 0)

## S4 method for signature 'MChromatograms'
removeIntensity(object, which = "below_threshold", threshold = 0)

## S4 method for signature 'XChromatogram'
removeIntensity(
  object,
  which = c("below_threshold", "outside_chromPeak"),
  threshold = 0
)
```

Arguments

`object`	an object representing chromatographic data. Can be a `Chromatogram()`, `MChromatograms()`, `XChromatogram()` or `XChromatograms()` object.
`which`	`character(1)` defining the condition to remove intensities. See description for details and options.
`threshold`	`numeric(1)` defining the threshold below which intensities are removed (if `which = "below_threshold"`).

Value

the input object with matching intensities being replaced by `NA`.

Author(s)

Johannes Rainer

Examples

```
library(MSnbase)
chr <- Chromatogram(rtime = 1:10 + rnorm(n = 10, sd = 0.3),
    intensity = c(5, 29, 50, NA, 100, 12, 3, 4, 1, 3))

## Remove all intensities below 20
res <- removeIntensity(chr, threshold = 20)
intensity(res)
```

retcor-methods *Correct retention time from different samples*

Description

To correct differences between retention times between different samples, a number of of methods exist in XCMS. `retcor` is the generic method.

Arguments

`object`	`xcmsSet-class` object
`method`	Method to use for retention time correction. See details.
`...`	Optional arguments to be passed along

Details

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

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

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

Value

An `xcmsSet` object with corrected retntion times.

Methods

object = "xcmsSet" `retcor(object, ...)`

See Also

`retcor.loess` `retcor.obiwarp` `xcmsSet-class`,

`retcor.obiwarp` *Align retention times across samples with Obiwarp*

Description

Calculate retention time deviations for each sample. It is based on the code at http://obi-warp.sourceforge.net/. However, this function is able to align multiple samples, by a center-star strategy.

For the original publication see

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

Arguments

`object`	the `xcmsSet` object
`plottype`	if `deviation` plot retention time deviation
`profStep`	step size (in m/z) to use for profile generation from the raw data files
`center`	the index of the sample all others will be aligned to. If center==NULL, the sample with the most peaks is chosen as default.
`col`	vector of colors for plotting each sample
`ty`	vector of line and point types for plotting each sample
`response`	Responsiveness of warping. 0 will give a linear warp based on start and end points. 100 will use all bijective anchors
`distFunc`	DistFunc function: cor (Pearson's R) or cor_opt (default, calculate only 10% diagonal band of distance matrix, better runtime), cov (covariance), prd (product), euc (Euclidean distance)
`gapInit`	Penalty for Gap opening, see below
`gapExtend`	Penalty for Gap enlargement, see below
`factorDiag`	Local weighting applied to diagonal moves in alignment.
`factorGap`	Local weighting applied to gap moves in alignment.
`localAlignment`	Local rather than global alignment
`initPenalty`	Penalty for initiating alignment (for local alignment only) Default: 0

Default gap penalties: (gapInit, gapExtend) [by distFunc type]: 'cor' = '0.3,2.4' 'cov' = '0,11.7' 'prd' = '0,7.8' 'euc' = '0.9,1.8'

Value

An `xcmsSet` object

Methods

object = "xcmsSet" retcor(object, method="obiwarp", plottype = c("none", "deviation"), profStep=1, center=NULL, col = NULL, ty = NULL, response=1, distFunc="cor_opt", gapInit=NULL, gapExtend=NULL, factorDiag=2, factorGap=1, localAlignment=0, initPenalty=0)

See Also

xcmsSet-class,

---

retcor.peakgroups-methods

Align retention times across samples

Description

These two methods use "well behaved" peak groups to calculate retention time deviations for every time point of each sample. Use smoothed deviations to align retention times.

Arguments

object	the xcmsSet object
missing	number of missing samples to allow in retention time correction groups
extra	number of extra peaks to allow in retention time correction correction groups
smooth	either "loess" for non-linear alignment or "linear" for linear alignment
span	degree of smoothing for local polynomial regression fitting
family	if gaussian fitting is by least-squares with no outlier removal, and if symmetric a re-descending M estimator is used with Tukey's biweight function, allowing outlier removal
plottype	if deviation plot retention time deviation points and regression fit, and if mdevden also plot peak overall peak density and retention time correction peak density
col	vector of colors for plotting each sample
ty	vector of line and point types for plotting each sample

Value

An xcmsSet object

Methods

object = "xcmsSet" `retcor(object, missing = 1, extra = 1, smooth = c("loess", "linear"), span = .2, family = c("gaussian", "symmetric"), plottype = c("none", "deviation", "mdevden"), col = NULL, ty = NULL)`

See Also

xcmsSet-class, loess retcor.obiwarp

retexp *Set retention time window to a specified width*

Description

Expands (or contracts) the retention time window in each row of a matrix as defined by the `retmin` and `retmax` columns.

Usage

```
retexp(peakrange, width = 200)
```

Arguments

`peakrange`	maxtrix with columns `retmin` and `retmax`
`width`	new width for the window

Value

The altered matrix.

Author(s)

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

See Also

`getEIC`

rla *Calculate relative log abundances*

Description

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

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)

rla(x, grp)
```

RsdFilter *Filter features based on their coefficient of variation*

Description

The 'RsdFilter' class and methods enable users to filter features from an 'XcmsExperiment' or 'SummarizedExperiment' object based on their relative standard deviation (coefficient of variation) for a specified threshold.

This 'filter' is part of the possible dispatch of the generic function 'filterFeatures'. Features *above* ('>') the user-input threshold will be removed from the entire dataset.

Usage

```
RsdFilter(threshold = 0.3, qcIndex = integer(), na.rm = TRUE, mad = FALSE)

## S4 method for signature 'XcmsResult,RsdFilter'
filterFeatures(object, filter, ...)

## S4 method for signature 'SummarizedExperiment,RsdFilter'
filterFeatures(object, filter, assay = 1)
```

Arguments

threshold	'numeric' value representing the threshold. Features with a coefficient of variation *strictly higher* ('>') than this will be removed from the entire dataset.
qcIndex	'integer' (or 'logical') vector corresponding to the indices of QC samples.
na.rm	'logical' indicates whether missing values ('NA') should be removed prior to the calculations.
mad	'logical' indicates whether the *Median Absolute Deviation* (MAD) should be used instead of the standard deviation. This is suggested for non-gaussian distributed data.
object	XcmsExperiment or SummarizedExperiment. For an XcmsExperiment object, the featureValues(object) will be evaluated, and for Summarizedesxperiment the assay(object, assay). The object will be filtered.
filter	The parameter object selecting and configuring the type of filtering. It can be one of the following classes: RsdFilter, DratioFilter, PercentMissingFilter or BlankFlag.
...	Optional parameters. For object being an XcmsExperiment: parameters for the featureValues() call.
assay	For filtering of SummarizedExperiment objects only. Indicates which assay the filtering will be based on. Note that the features for the entire object will be removed, but the computations are performed on a single assay. Default is 1, which means the first assay of the object will be evaluated.

Value

For 'RsdFilter': a 'RsdFilter' class. 'filterFeatures' return the input object minus the features that did not met the user input threshold.

Note

It is assumed that the abundance values are in natural scale. Abundances in log scale should be first transformed to natural scale before calculating the RSD.

Author(s)

Philippine Louail

See Also

Other Filter features in xcms: BlankFlag, DratioFilter, PercentMissingFilter

---

sampnames-methods *Get sample names*

Description

Return sample names for an object

Value

A character vector with sample names.

Methods

object = "xcmsEIC" sampnames(object)

object = "xcmsSet" sampnames(object)

See Also

xcmsSet-class, xcmsEIC-class

---

showError,xcmsSet-method *Extract processing errors*

Description

If peak detection is performed with findPeaks setting argument stopOnError = FALSE eventual errors during the process do not cause to stop the processing but are recorded inside of the resulting xcmsSet object. These errors can be accessed with the showError method.

Usage

```
## S4 method for signature 'xcmsSet'
showError(object, message. = TRUE, ...)
```

Arguments

object	An xcmsSet object.
message.	Logical indicating whether only the error message, or the error itself should be returned.
...	Additional arguments.

Value

A list of error messages (if `message. = TRUE`) or errors or an empty list if no errors are present.

Author(s)

Johannes Rainer

`specDist-methods` *Distance methods for xcmsSet, xcmsRaw and xsAnnotate*

Description

There are several methods for calculating a distance between two sets of peaks in xcms. `specDist` is the generic method.

Arguments

`object`	a xcmsSet or xcmsRaw.
`method`	Method to use for distance calculation. See details.
`...`	mzabs, mzppm and parameters for the distance function.

Details

Different algorithms can be used by specifying them with the `method` argument. For example to use the "meanMZmatch" approach with xcmsSet one would use: `specDist(object, peakIDs1, peakIDs2, method="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

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

Methods

object = "xcmsSet" `specDist(object, peakIDs1, peakIDs2,...)`

object = "xsAnnotate" `specDist(object, PSpec1, PSpec2,...)`

Author(s)

Joachim Kutzera, <jkutzer@ipb-halle.de>

specDist.cosine *a Distance function based on matching peaks*

Description

This method calculates the distance of two sets of peaks using the cosine-distance.

Usage

```
specDist.cosine(peakTable1, peakTable2, mzabs=0.001, mzppm=10, mzExp=0.6,
                intExp=3, nPdiff=2, nPmin=8, 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
mzExp	the exponent used for mz
intExp	the exponent used for intensity
nPdiff	the maximum nrow-difference of the two peaktables
nPmin	the minimum absolute sum of peaks from both praktables

Details

The result is the cosine-distance of the product from weighted factors of mz and intensity from matching peaks in the two peaktables. The factors are calculated as wFact = mz^mzExp * int^intExp. if no distance is calculated (for example because no matching peaks were found) the return-value is NA.

Methods

peakTable1 = "matrix", peakTable2 = "matrix" `specDist.cosine(peakTable1, peakTable2, mzabs = 0.001, mzppm = 10, mzExp = 0.6, intExp = 3, nPdiff = 2, nPmin = 8, symmetric = FALSE)`

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, symmetric=TRUE)
```

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, matchdist=1, matchrate=1, mzabs=0.001, mzppm=10, symmetric=TRUE)`

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=10,symmetric=FALSE )`

Author(s)

Joachim Kutzera, <jkutzer@ipb-halle.de>

specNoise

Calculate noise for a sparse continuum mass spectrum

Description

Given a sparse continuum mass spectrum, determine regions where no signal is present, substituting half of the minimum intensity for those regions. Calculate the noise level as the weighted mean of the regions with signal and the regions without signal. If there is only one raw peak, return zero.

Usage

```
specNoise(spec, gap = quantile(diff(spec[, "mz"]), 0.9))
```

Arguments

spec	matrix with named columns mz and intensity
gap	threshold above which to data points are considerd to be separated by a blank region and not bridged by an interpolating line

Details

The default gap value is determined from the 90th percentile of the pair-wise differences between adjacent mass values.

Value

A numeric noise level

Author(s)

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

See Also

getSpec, specPeaks

---

specPeaks *Identify peaks in a sparse continuum mode spectrum*

Description

Given a spectrum, identify and list significant peaks as determined by several criteria.

Usage

```
specPeaks(spec, sn = 20, mzgap = 0.2)
```

Arguments

spec	matrix with named columns mz and intensity
sn	minimum signal to noise ratio
mzgap	minimal distance between adjacent peaks, with smaller peaks being excluded

Details

Peaks must meet two criteria to be considered peaks: 1) Their s/n ratio must exceed a certain threshold. 2) They must not be within a given distance of any greater intensity peaks.

Value

A matrix with columns:

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

Author(s)

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

See Also

getSpec, specNoise

---

split.xcmsRaw *Divide an xcmsRaw object*

Description

Divides the scans from a xcmsRaw object into a list of multiple objects. MS^n data is discarded.

Arguments

x	xcmsRaw object
f	factor such that factor(f) defines the scans which go into the new xcmsRaw objects
drop	logical indicating if levels that do not occur should be dropped (if 'f' is a 'factor' or a list).
...	further potential arguments passed to methods.

Value

A list of xcmsRaw objects.

Methods

xr = "xcmsRaw" `split(x, f, drop = TRUE, ...)`

Author(s)

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

See Also

xcmsRaw-class

split.xcmsSet *Divide an xcmsSet object*

Description

Divides the samples and peaks from a xcmsSet object into a list of multiple objects. Group data is discarded.

Arguments

xs	xcmsSet object
f	factor such that factor(f) defines the grouping
drop	logical indicating if levels that do not occur should be dropped (if 'f' is a 'factor' or a list).
...	further potential arguments passed to methods.

Value

A list of xcmsSet objects.

Methods

xs = "xcmsSet" `split(x, f, drop = TRUE, ...)`

Author(s)

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

See Also

xcmsSet-class

SSgauss *Gaussian Model*

Description

This selfStart model evalueates the Gaussian model and its gradient. It has an initial attribute that will evalueate the inital estimates of the parameters mu, sigma, and h.

Usage

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

Arguments

x	a numeric vector of values at which to evaluate the model
mu	mean of the distribution function
sigma	standard deviation of the distribution fuction
h	height of the distribution function

Details

Initial values for mu and h are chosen from the maximal value of x. The initial value for sigma is determined from the area under x divided by h*sqrt(2*pi).

Value

A numeric vector of the same length as x. It is the value of the expression h*exp(-(x-mu)^2/(2*sigma^2), which is a modified gaussian function where the maximum height is treated as a separate parameter not dependent on sigma. If arguments mu, sigma, and h are names of objects, the gradient matrix with respect to these names is attached as an attribute named gradient.

Author(s)

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

See Also

nls, selfStart

---

stitch-methods *Correct gaps in data*

Description

Fixes gaps in data due to calibration scans or lock mass. Automatically detects file type and calls the relevant method. The mzXML file keeps the data the same length in time but overwrites the lock mass scans. The netCDF version adds the scans back into the data thereby increasing the length of the data and correcting for the unseen gap.

Arguments

object	An xcmsRaw-class object
lockMass	A dataframe of locations of the gaps
freq	The intervals of the lock mass scans
start	The starting lock mass scan location, default is 1

Details

makeacqNum takes locates the gap using the starting lock mass scan and it's intervals. This data frame is then used in stitch to correct for the gap caused by the lock mass. Correction works by using scans from either side of the gap to fill it in.

Value

stitch A corrected xcmsRaw-class object makeacqNum A numeric vector of scan locations corresponding to lock Mass scans

Methods

object = "xcmsRaw" `stitch(object, lockMass=numeric())`

object = "xcmsRaw" `makeacqNum(object, freq=numeric(), start=1)`

Author(s)

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

Examples

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

    ## plot the old data before correction
    foo<-rawEIC(xr, m=c(200,210), scan=c(80,140))
    plot(foo$scan, foo$intensity, type="h")

    ## plot the new corrected data to see what changed
    foo<-rawEIC(ob, m=c(200,210), scan=c(80,140))
    plot(foo$scan, foo$intensity, type="h")

## End(Not run)
```

storeResults *Save xcms result objects in a specified format*

Description

The storeResults function saves an object resulting from processing with the xcms package (mainly XcmsExperiment). Multiple formats for storing and exporting are available and can be defined by the param argument.

Supported param objects are:

- RDataParam: Save in an .RData format file. The name of the file can be specified in the fileName argument.
- PlainTextParam: Store MsExperiment and XcmsExperiment objects as a folder of plain text files, folder path defined in the path argument.
- MzTabMParam: Save in MzTab format (to be defined).

For specific examples, see the help pages of the individual parameter classes listed above.

Usage

```
storeResults(object, param, ...)
```

Arguments

object	MsExperiment or XcmsExperiment The data object that needs to be saved.
param	The parameter object selecting and configuring the format for saving. It can be one of the following classes: RDataParam, PlainTextParam, or MzTabMParam.
...	Optional parameters.

Author(s)

Philippine Louail

Examples

```
## Load a test data set with detected peaks
library(xcms)
library(MsExperiment)
faahko_sub <- loadXcmsData("faahko_sub2")

## Set up parameter to save as .RData file
param <- RDataParam(fileName = "example_xcms_results")

## save as .RData
storeResults(object = faahko_sub, param = param)

## Set up parameter to save as a collection of plain text file
param <- PlainTextParam(path = "test/path/")
```

```
## Save as a collection of plain text files
storeResults(object = faahko_sub, param = param)
```

`updateObject,xcmsSet-method` *Update an* `xcmsSet` *object*

Description

This method updates an *old* `xcmsSet` object to the latest definition.

Usage

```
## S4 method for signature 'xcmsSet'
updateObject(object, ..., verbose = FALSE)
```

Arguments

`object`	The `xcmsSet` object to update.
`...`	Optional additional arguments. Currently ignored.
`verbose`	Currently ignored.

Value

An updated `xcmsSet` containing all data from the input object.

Author(s)

Johannes Rainer

`useOriginalCode` *Enable usage of old xcms code*

Description

This function allows to enable the usage of old, partially deprecated code from xcms by setting a corresponding global option. See details for functions affected.

Usage

```
useOriginalCode(x)
```

Arguments

x	`logical(1)` to specify whether or not original old code should be used in corresponding functions. If not provided the function simply returns the value of the global option.

Details

The functions/methods that 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 matchedFilter 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 dicouraged. This function is thought to be used mainly in the transition phase from xcms to xcms version 3.

Author(s)

Johannes Rainer

`verify.mzQuantM` *Verify an mzQuantML file*

Description

Export in XML data formats: verify the written data

Usage

```
verify.mzQuantML(filename, xsdfilename)
```

Arguments

filename	filename (may include full path) for the output file. Pipes or URLs are not allowed.
xsdfilename	Filename of the XSD to verify against (may include full path)

Details

The verify.mzQuantML() function will verify an PSI standard format mzQuantML document against the XSD schemda, see http://www.psidev.info/mzquantml

Value

None.

See Also

write.mzQuantML

---

write.cdf-methods *Save an xcmsRaw object to file*

Description

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

Arguments

object	the xcmsRaw object
filename	filename (may include full path) for the CDF file. Pipes or URLs are not allowed.

Details

Currently the only application known to read the resulting file is XCMS. Others, especially those which build on the AndiMS library, will refuse to load the output.

Value

None.

Methods

object = "xcmsRaw" `write.cdf(object, filename)`

See Also

xcmsRaw-class, xcmsRaw,

write.mzdata-methods *Save an xcmsRaw object to a file*

Description

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

Arguments

object	the xcmsRaw object
filename	filename (may include full path) for the mzData file. Pipes or URLs are not allowed.

Details

This function will export a given xcmsRaw object to an mzData file. The mzData file will contain a <spectrumList> containing the <spectrum> with mass and intensity values in 32 bit precision. Other formats are currently not supported. Any header information (e.g. additional <software> information or <cvParams>) will be lost. Currently, also any MSn information will not be stored.

Value

None.

Methods

object = "xcmsRaw" `write.mzdata(object, filename)`

See Also

xcmsRaw-class, xcmsRaw,

write.mzQuantML-methods *Save an xcmsSet object to an PSI mzQuantML file*

Description

Export in XML data formats: Write the processed data in an xcmsSet to mzQuantML.

Arguments

object	the xcmsRaw or xcmsSet object
filename	filename (may include full path) for the output file. Pipes or URLs are not allowed.

Details

The write.mzQuantML() function will write a (grouped) xcmsSet into the PSI standard format mzQuantML, see http://www.psidev.info/mzquantml

Value

None.

Methods

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

See Also

xcmsSet-class, xcmsSet, verify.mzQuantML,

---

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

`object`
: the `xcmsSet` object

`filename`
: filename (may include full path) for the mzTab file. Pipes or URLs are not allowed.

Details

The mzTab file format for MS-based metabolomics (and proteomics) is a lightweight supplement to the existing standard XML-based file formats (mzML, mzIdentML, mzQuantML), providing a comprehensive summary, similar in concept to the supplemental material of a scientific publication. mzTab files from xcms contain small molecule sections together with experimental metadata and basic quantitative information. The format is intended to store a simple summary of the final results.

Value

None.

Usage

object = "xcmsSet" `writeMzTab(object, filename)`

See Also

`xcmsSet-class`, `xcmsSet`,

Examples

```
library(faahKO)
xs <- group(faahko)

mzt <- data.frame(character(0))
mzt <- xcms:::mzTabHeader(mzt,
                  version="1.1.0", mode="Complete", type="Quantification",
                  description="faahKO",
                  xset=xs)
mzt <- xcms:::mzTabAddSME(mzt, xs)

xcms:::writeMzTab(mzt, "faahKO.mzTab")
```

XChromatograms *Containers for chromatographic and peak detection data*

Description

The XChromatogram object allows to store chromatographic data (e.g. an extracted ion chromatogram) along with identified chromatographic peaks within that data. The object inherits all functions from the Chromatogram() object in the MSnbase package.

Multiple XChromatogram objects can be stored in a XChromatograms object. This class extends MChromatograms() from the MSnbase package and allows thus to arrange chromatograms in a matrix-like structure, columns representing samples and rows m/z-retention time ranges.

All functions are described (grouped into topic-related sections) after the **Arguments** section.

Usage

```
XChromatograms(data, phenoData, featureData, chromPeaks, chromPeakData, ...)

XChromatogram(
  rtime = numeric(),
  intensity = numeric(),
  mz = c(NA_real_, NA_real_),
  filterMz = c(NA_real_, NA_real_),
  precursorMz = c(NA_real_, NA_real_),
  productMz = c(NA_real_, NA_real_),
  fromFile = integer(),
  aggregationFun = character(),
  msLevel = 1L,
  chromPeaks,
  chromPeakData
)

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

```
## S4 method for signature 'XChromatogram'
chromPeaks(
  object,
  rt = numeric(),
  mz = numeric(),
  ppm = 0,
  type = c("any", "within", "apex_within"),
  msLevel
)

## S4 replacement method for signature 'XChromatogram'
chromPeaks(object) <- value

## S4 method for signature 'XChromatogram,ANY'
plot(
  x,
  col = "#00000060",
  lty = 1,
  type = "l",
  xlab = "retention time",
  ylab = "intensity",
  main = NULL,
  peakType = c("polygon", "point", "rectangle", "none"),
  peakCol = "#00000060",
  peakBg = "#00000020",
  peakPch = 1,
  ...
)

## S4 method for signature 'XChromatogram'
filterMz(object, mz, ...)

## S4 method for signature 'XChromatogram'
filterRt(object, rt, ...)

## S4 method for signature 'XChromatogram'
hasChromPeaks(object)

## S4 method for signature 'XChromatogram'
dropFilledChromPeaks(object)

## S4 method for signature 'XChromatogram'
chromPeakData(object)

## S4 replacement method for signature 'XChromatogram'
chromPeakData(object) <- value

## S4 method for signature 'XChromatogram,MergeNeighboringPeaksParam'
```

```
refineChromPeaks(object, param = MergeNeighboringPeaksParam())

## S4 method for signature 'XChromatogram'
filterChromPeaks(object, method = c("keepTop"), ...)

## S4 method for signature 'XChromatogram'
transformIntensity(object, FUN = identity)

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

## S4 method for signature 'XChromatograms'
hasChromPeaks(object)

## S4 method for signature 'XChromatograms'
hasFilledChromPeaks(object)

## S4 method for signature 'XChromatograms'
chromPeaks(
  object,
  rt = numeric(),
  mz = numeric(),
  ppm = 0,
  type = c("any", "within", "apex_within"),
  msLevel
)

## S4 method for signature 'XChromatograms'
chromPeakData(object)

## S4 method for signature 'XChromatograms'
filterMz(object, mz, ...)

## S4 method for signature 'XChromatograms'
filterRt(object, rt, ...)

## S4 method for signature 'XChromatograms,ANY'
plot(
  x,
  col = "#00000060",
  lty = 1,
  type = "l",
  xlab = "retention time",
  ylab = "intensity",
  main = NULL,
  peakType = c("polygon", "point", "rectangle", "none"),
  peakCol = "#00000060",
  peakBg = "#00000020",
```

```
  peakPch = 1,
  ...
)

## S4 method for signature 'XChromatograms'
processHistory(object, fileIndex, type)

## S4 method for signature 'XChromatograms'
hasFeatures(object, ...)

## S4 method for signature 'XChromatograms'
dropFeatureDefinitions(object, ...)

## S4 method for signature 'XChromatograms,PeakDensityParam'
groupChromPeaks(object, param)

## S4 method for signature 'XChromatograms'
featureDefinitions(
  object,
  mz = numeric(),
  rt = numeric(),
  ppm = 0,
  type = c("any", "within", "apex_within")
)

## S4 method for signature 'XChromatograms,ANY,ANY,ANY'
x[i, j, drop = TRUE]

## S4 method for signature 'XChromatograms'
featureValues(
  object,
  method = c("medret", "maxint", "sum"),
  value = "into",
  intensity = "into",
  missing = NA,
  ...
)

## S4 method for signature 'XChromatograms'
plotChromPeakDensity(
  object,
  param,
  col = "#00000060",
  xlab = "retention time",
  main = NULL,
  peakType = c("polygon", "point", "rectangle", "none"),
  peakCol = "#00000060",
  peakBg = "#00000020",
```

```
  peakPch = 1,
  simulate = TRUE,
  ...
)

## S4 method for signature 'XChromatograms'
dropFilledChromPeaks(object)

## S4 method for signature 'XChromatograms,MergeNeighboringPeaksParam'
refineChromPeaks(object, param = MergeNeighboringPeaksParam())

## S4 method for signature 'XChromatograms'
filterChromPeaks(object, method = c("keepTop"), ...)

## S4 method for signature 'XChromatograms'
transformIntensity(object, FUN = identity)
```

Arguments

data	For XChromatograms: list of Chromatogram or XChromatogram objects.
phenoData	For XChromatograms: either a data.frame, AnnotatedDataFrame or NAnnotatedDataFrame describing the phenotypical information of the samples.
featureData	For XChromatograms: either a data.frame or AnnotatedDataFrame with additional information for each row of chromatograms.
chromPeaks	For XChromatogram: matrix with required columns "rt", "rtmin", "rtmax", "into", "maxo" and "sn". For XChromatograms: list, same length than data, with the chromatographic peaks for each chromatogram. Each element has to be a matrix, the ordering has to match the order of the chromatograms in data.
chromPeakData	For XChromatogram: DataFrame with optional additional annotations for each chromatographic peak. The number of rows has to match the number of chromatographic peaks.
...	For filterChromPeaks: additional parameters defining how to filter chromatographic peaks. See function description below for details.
rtime	For XChromatogram: numeric with the retention times (length has to be equal to the length of intensity).
intensity	For XChromatogram: numeric with the intensity values (length has to be equal to the length of rtime). For `featureValues`: `character(1)` specifying the name of the column in `chromPeaks(object)` containing the intensity value of the peak that should be used for the `method = "maxint"` conflict resolution if.
mz	For XChromatogram: numeric(2) representing the m/z value range (min, max) on which the chromatogram was created. This is supposed to contain the *real* range of m/z values in contrast to the filterMz below. For chromPeaks and

featureDefinitions: numeric(2) defining the m/z range for which chromatographic peaks or features should be returned. For filterMz: numeric(2) defining the m/z range for which chromatographic peaks should be retained.#'

filterMz — For XChromatogram: numeric(2) representing the m/z value range (min, max) that was used to filter the original object on m/z dimension. If not applicable use filterMz = c(0, 0).

precursorMz — For XChromatogram: numeric(2) for SRM/MRM transitions. Represents the mz of the precursor ion. See details for more information.

productMz — For XChromatogram: numeric(2) for SRM/MRM transitions. Represents the mz of the product. See details for more information.

fromFile — For XChromatogram: integer(1) the index of the file within the OnDiskMSnExp or MSnExp object from which the chromatogram was extracted.

aggregationFun — For XChromatogram: character(1) specifying the function that was used to aggregate intensity values for the same retention time across the m/z range.

msLevel — For XChromatogram: integer with the MS level from which the chromatogram was extracted. For chromPeaks and chromPeakData: extract chromatographic peaks of a certain MS level.

object — An XChromatogram or XChromatograms object.

rt — For chromPeaks and featureDefinitions: numeric(2) defining the retention time range for which chromatographic peaks or features should be returned. For filterRt: numeric(2) defining the retention time range to reduce object to.

ppm — For chromPeaks and featureDefinitions: numeric(1) defining a ppm to expand the provided m/z range.

type — For chromPeaks and featureDefinitions: character(1) defining which peaks or features to return if rt or mz is provided: "any" (default) return all peaks that are even partially overlapping with rt, "within" return peaks that are completely within rt and "apex_within" return peaks which apex is within rt.

For `plot`: what type of plot should be used for the chromatogram (such as `"l"` for lines, `"p"` for points etc), see help of [plot()] in the `graphics` package for more details.
For `processHistory`: restrict returned processing steps to specific types. Use [processHistoryTypes()] to list all supported values.

value — For chromPeaks<-: a numeric matrix with required columns "rt", "rtmin", "rtmax", "into" and "maxo".

For `featureValues`: `character(1)` specifying the name of the column in `chromPeaks(object)` that should be returned or `"index"` (default) to return the index of the peak associated with the feature in each sample. To return the integrated peak area instead of the index use `value = "into"`.

x — For plot: an XChromatogram or XChromatograms object.

col — For plot: the color to be used to draw the chromatogram.

lty — For plot and plotChromPeakDensity: the line type.

xlab — For plot and plotChromPeakDensity: the x axis label.

ylab — For plot: the y axis label.

main — For plot and plotChromPeakDensity: an optional title for the plot.

peakType — For plot and plotChromPeakDensity: character(1) defining how (and if) identified chromatographic peak within the chromatogram should be plotted. Options are "polygon" (default): draw the peak borders with the peakCol color and fill the peak area with the peakBg color, "point": indicate the peak's apex with a point, "rectangle": draw a rectangle around the identified peak and "none": don't draw peaks.

peakCol — For plot and plotChromPeakDensity: the foreground color for the peaks. For peakType = "polygon" and peakType = "rectangle" this is the color for the border. Use NA to not use a foreground color. This should either be a single color or a vector of colors with the same length than chromPeaks(x) has rows.

peakBg — For plot and plotChromPeakDensity: the background color for the peaks. For peakType = "polygon" and peakType = "rectangle" the peak are or rectangle will be filled with this color. Use NA to skip. This should be either a single color or a vector of colors with the same length than chromPeaks(x) has rows.

peakPch — For plot and plotChromPeakDensity: the point character to be used for peakType = "point". See plot() in the graphics package for more details.

param — For groupChromPeaks and plotChromPeakDensity: a PeakDensityParam() object with the settings for the *peak density* correspondence analysis algorithm.

method — For featureValues: character(1) specifying the method to resolve multi-peak mappings within the sample sample, i.e. to select the *representative* peak for a feature for which more than one peak was assigned in one sample. Options are "medret" (default): select the peak closest to the median retention time of the feature, "maxint": select the peak with the largest signal and "sum": sum the values of all peaks (only if value is "into" or "maxo"). For filterChromPeaks: character(1) defining the method that should be used to filter chromatographic peaks. See help on filterChromPeaks below for details.

FUN — For transformIntensity: a function to transform the intensity values of object.

fileIndex — For processHistory: optional integer specifying the index of the files/samples for which the ProcessHistory objects should be returned.

i — For [: integer with the row indices to subset the XChromatograms object.

j — For [: integer with the column indices to subset the XChromatograms object.

drop — For [: logical(1) whether the dimensionality should be dropped (if possible). Defaults to drop = TRUE, thus, if length of i and j is 1 a XChromatogram is returned. Note that drop is ignored if length of i or j is larger than 1, thus a XChromatograms is returned.

missing — For featureValues: how missing values should be reported. Allowed values are NA (default), a numeric(1) to replace NAs with that value or missing = "rowmin_half" to replace NAs with half of the row's minimal (non-missing) value.

simulate — For plotChromPeakDensity: logical(1) whether a correspondence analysis should be *simulated* based on the available data and the provided PeakDensityParam() param argument. See section *Correspondence analysis* for details.

Value

See help of the individual functions.

Creation of objects

Objects can be created with the contructor function `XChromatogram` and `XChromatograms`, respectively. Also, they can be coerced from Chromatogram or `MChromatograms()` objects using `as(object, "XChromatogram")` or `as(object, "XChromatograms")`.

Filtering and subsetting

Besides classical subsetting with `[` specific filter operations on `MChromatograms()` and `XChromatograms` objects are available. See `filterColumnsIntensityAbove()` for more details.

- `[` allows to subset a `XChromatograms` object by row (`i`) and column (`j`), with `i` and `j` being of type `integer`. The `featureDefinitions` will also be subsetted accordingly and the `peakidx` column updated.
- `filterMz` filters the chromatographic peaks within an `XChromatogram` or `XChromatograms`, if a column `"mz"` is present in the `chromPeaks` matrix. This would be the case if the `XChromatogram` was extracted from an `XCMSnExp()` object with the `chromatogram()` function. All chromatographic peaks with their m/z within the m/z range defined by `mz` will be retained. Also feature definitions (if present) will be subset accordingly. The function returns a filtered `XChromatogram` or `XChromatograms` object.
- `filterRt` filters chromatogram(s) by the provided retention time range. All eventually present chromatographic peaks with their apex within the retention time range specified with `rt` will be retained. Also feature definitions, if present, will be filtered accordingly. The function returns a filtered `XChromatogram` or `XChromatograms` object.

Accessing data

See also help of Chromatogram in the `MSnbase` package for general information and data access. The methods listed here are specific for `XChromatogram` and `XChromatograms` objects.

- `chromPeaks`, `chromPeaks<-`: extract or set the matrix with the chromatographic peak definitions. Parameter `rt` allows to specify a retention time range for which peaks should be returned along with parameter `type` that defines how *overlapping* is defined (parameter description for details). For `XChromatogram` objects the function returns a `matrix` with columns `"rt"` (retention time of the peak apex), `"rtmin"` (the lower peak boundary), `"rtmax"` (the upper peak boundary), `"into"` (the ingegrated peak signal/area of the peak), `"maxo"` (the maximum instensity of the peak and `"sn"` (the signal to noise ratio). Note that, depending on the peak detection algorithm, the matrix may contain additional columns. For `XChromatograms` objects the `matrix` contains also columns `"row"` and `"column"` specifying in which chromatogram of `object` the peak was identified. Chromatographic peaks are ordered by row.
- `chromPeakData`, `chromPeakData<-`: extract or set the `DataFrame()` with optional chromatographic peak annotations.
- `hasChromPeaks`: infer whether a `XChromatogram` (or `XChromatograms`) has chromatographic peaks. For `XChromatogram`: returns a `logical(1)`, for `XChromatograms`: returns a `matrix`, same dimensions than `object` with either `TRUE` or `FALSE` if chromatographic peaks are available in the chromatogram at the respective position.

- hasFilledChromPeaks: whether a XChromatogram (or a XChromatogram in a XChromatograms) has filled-in chromatographic peaks. For XChromatogram: returns a logical(1), for XChromatograms: returns a matrix, same dimensions than object with either TRUE or FALSE if chromatographic peaks are available in the chromatogram at the respective position.
- dropFilledChromPeaks: removes filled-in chromatographic peaks. See dropFilledChromPeaks() help for XCMSnExp() objects for more information.
- hasFeatures: for XChromatograms objects only: if correspondence analysis has been performed and m/z-rt feature definitions are present. Returns a logical(1).
- dropFeatureDefinitions: for XChrmomatograms objects only: delete any correspondence analysis results (and related process history).
- featureDefinitions: for XChromatograms objects only. Extract the results from the correspondence analysis (performed with groupChromPeaks). Returns a DataFrame with the properties of the defined m/z-rt features: their m/z and retention time range. Columns peakidx and row contain the index of the chromatographic peaks in the chromPeaks matrix associated with the feature and the row in the XChromatograms object in which the feature was defined. Similar to the chromPeaks method it is possible to filter the returned feature matrix with the mz, rt and ppm parameters.
- featureValues: for XChromatograms objects only. Extract the abundance estimates for the individuals features. Note that by default (with parameter value = "index" a matrix of indices of the peaks in the chromPeaks matrix associated to the feature is returned. To extract the integrated peak area use value = "into". The function returns a matrix with one row per feature (in featureDefinitions) and each column being a sample (i.e. column of object). For features without a peak associated in a certain sample NA is returned. This can be changed with the missing argument of the function.
- filterChromPeaks: *filters* chromatographic peaks in object depending on parameter method and method-specific parameters passed as additional arguments with .... Available methods are:
  - method = "keepTop": keep top n (default n = 1L) peaks in each chromatogram ordered by column order (defaults to order = "maxo"). Parameter decreasing (default decreasing = TRUE) can be used to order peaks in descending (decreasing = TRUE) or ascending (decreasing = FALSE) order to keep the top n peaks with largest or smallest values, respectively.
- processHistory: returns a list of ProcessHistory objects representing the individual performed processing steps. Optional parameters type and fileIndex allow to further specify which processing steps to return.

Manipulating data

- transformIntensity: transforms the intensity values of the chromatograms with provided function FUN. See transformIntensity() in the MSnbase package for details. For XChromatogram and XChromatograms in addition to the intensity values also columns "into" and "maxo" in the object's chromPeaks matrix are transformed by the same function.

Plotting and visualizing

- plot draws the chromatogram and highlights in addition any chromatographic peaks present in the XChromatogram or XChromatograms (unless peakType = "none" was specified). To

draw peaks in different colors a vector of color definitions with length equal to `nrow(chromPeaks(x))` has to be submitted with `peakCol` and/or `peakBg` defining one color for each peak (in the order as peaks are in `chromPeaks(x)`). For base peak chromatograms or total ion chromatograms it might be better to set `peakType = "none"` to avoid generating busy plots.

- `plotChromPeakDensity`: visualize *peak density*-based correspondence analysis results. See section *Correspondence analysis* for more details.

Chromatographic peak detection

See findChromPeaks-Chromatogram-CentWaveParam for information.

After chromatographic peak detection it is also possible to *refine* identified chromatographic peaks with the `refineChromPeaks` method (e.g. to reduce peak detection artifacts). Currently, only peak refinement using the *merge neighboring peaks* method is available (see `MergeNeighboringPeaksParam()` for a detailed description of the approach.

Correspondence analysis

Identified chromatographic peaks in an `XChromatograms` object can be grouped into *features* with the `groupChromPeaks` function. Currently, such a correspondence analysis can be performed with the *peak density* method (see groupChromPeaks for more details) specifying the algorithm settings with a `PeakDensityParam()` object. A correspondence analysis is performed separately for each row in the `XChromatograms` object grouping chromatographic peaks across samples (columns).

The analysis results are stored in the returned `XChromatograms` object and can be accessed with the `featureDefinitions` method which returns a `DataFrame` with one row for each feature. Column `"row"` specifies in which row of the `XChromatograms` object the feature was identified.

The `plotChromPeakDensity` method can be used to visualize *peak density* correspondence results, or to *simulate* a peak density correspondence analysis on chromatographic data. The resulting plot consists of two panels, the upper panel showing the chromatographic data as well as the identified chromatographic peaks, the lower panel the distribution of peaks (the peak density) along the retention time axis. This plot shows each peak as a point with it's peak's retention time on the x-axis, and the sample in which it was found on the y-axis. The distribution of peaks along the retention time axis is visualized with a density estimate. Grouped chromatographic peaks are indicated with grey shaded rectangles. Parameter `simulate` allows to define whether the correspondence analysis should be simulated (`simulate=TRUE`, based on the available data and the provided `PeakDensityParam()` parameter class) or not (`simulate=FALSE`). For the latter it is assumed that a correspondence analysis has been performed with the *peak density* method on the `object`. See examples below.

Abundance estimates for each feature can be extracted with the `featureValues` function using parameter `value = "into"` to extract the integrated peak area for each feature. The result is a `matrix`, columns being samples and rows features.

Note

Highlighting the peak area(s) in an `XChromatogram` or `XChromatograms` object (`plot` with `peakType = "polygon"`) draws a polygon representing the displayed chromatogram from the peak's minimal retention time to the maximal retention time. If the `XChromatograms` was extracted from an `XCMSnExp()` object with the `chromatogram()` function this might not represent the actual identified peak area if the m/z range that was used to extract the chromatogram was larger than the peak's m/z.

Author(s)

Johannes Rainer

See Also

findChromPeaks-centWave for peak detection on `MChromatograms()` objects.

Examples

```
## ---- Creation of XChromatograms ----
##
## Create a XChromatograms from Chromatogram objects
library(MSnbase)
dta <- list(Chromatogram(rtime = 1:7, c(3, 4, 6, 12, 8, 3, 2)),
    Chromatogram(1:10, c(4, 6, 3, 4, 7, 13, 43, 34, 23, 9)))

## Create an XChromatograms without peak data
xchrs <- XChromatograms(dta)

## Create an XChromatograms with peaks data
pks <- list(matrix(c(4, 2, 5, 30, 12, NA), nrow = 1,
    dimnames = list(NULL, c("rt", "rtmin", "rtmax", "into", "maxo", "sn"))),
    NULL)
xchrs <- XChromatograms(dta, chromPeaks = pks)

## Create an XChromatograms from XChromatogram objects
dta <- lapply(dta, as, "XChromatogram")
chromPeaks(dta[[1]]) <- pks[[1]]

xchrs <- XChromatograms(dta, nrow = 1)

hasChromPeaks(xchrs)

## Loading a test data set with identified chromatographic peaks
faahko_sub <- loadXcmsData("faahko_sub2")

## Subset the dataset to the first and third file.
xod_sub <- filterFile(faahko_sub, file = c(1, 3))

od <- as(xod_sub, "MsExperiment")

## Extract chromatograms for a m/z - retention time slice
chrs <- chromatogram(od, mz = 344, rt = c(2500, 3500))
chrs

## ------------------------------------------------- ##
##       Chromatographic peak detection              ##
## ------------------------------------------------- ##
## Perform peak detection using CentWave
xchrs <- findChromPeaks(chrs, param = CentWaveParam())
xchrs
```

```
## Do we have chromatographic peaks?
hasChromPeaks(xchrs)

## Process history
processHistory(xchrs)

## The chromatographic peaks, columns "row" and "column" provide information
## in which sample the peak was identified.
chromPeaks(xchrs)

## Spectifically extract chromatographic peaks for one sample/chromatogram
chromPeaks(xchrs[1, 2])

## Plot the results
plot(xchrs)

## Plot the results using a different color for each sample
sample_colors <- c("#ff000040", "#00ff0040", "#0000ff40")
cols <- sample_colors[chromPeaks(xchrs)[, "column"]]
plot(xchrs, col = sample_colors, peakBg = cols)

## Indicate the peaks with a rectangle
plot(xchrs, col = sample_colors, peakCol = cols, peakType = "rectangle",
    peakBg = NA)

## ------------------------------------------------- ##
##       Correspondence analysis                     ##
## ------------------------------------------------- ##
## Group chromatographic peaks across samples
prm <- PeakDensityParam(sampleGroup = rep(1, 2))
res <- groupChromPeaks(xchrs, param = prm)

hasFeatures(res)
featureDefinitions(res)

## Plot the correspondence results. Use simulate = FALSE to show the
## actual results. Grouped chromatographic peaks are indicated with
## grey shaded rectangles.
plotChromPeakDensity(res, simulate = FALSE)

## Simulate a correspondence analysis based on different settings. Larger
## bw will increase the smoothing of the density estimate hence grouping
## chromatographic peaks that are more apart on the retention time axis.
prm <- PeakDensityParam(sampleGroup = rep(1, 3), bw = 60)
plotChromPeakDensity(res, param = prm)

## Delete the identified feature definitions
res <- dropFeatureDefinitions(res)
hasFeatures(res)

library(MSnbase)
## Create a XChromatogram object
pks <- matrix(nrow = 1, ncol = 6)
```

```
colnames(pks) <- c("rt", "rtmin", "rtmax", "into", "maxo", "sn")
pks[, "rtmin"] <- 2
pks[, "rtmax"] <- 9
pks[, "rt"] <- 4
pks[, "maxo"] <- 19
pks[, "into"] <- 93

xchr <- XChromatogram(rtime = 1:10,
    intensity = c(4, 8, 14, 19, 18, 12, 9, 8, 5, 2),
    chromPeaks = pks)
xchr

## Add arbitrary peak annotations
df <- DataFrame(peak_id = c("a"))
xchr <- XChromatogram(rtime = 1:10,
    intensity = c(4, 8, 14, 19, 18, 12, 9, 8, 5, 2),
    chromPeaks = pks, chromPeakData = df)
xchr
chromPeakData(xchr)

## Extract the chromatographic peaks
chromPeaks(xchr)

## Plotting of a single XChromatogram object
## o Don't highlight chromatographic peaks
plot(xchr, peakType = "none")

## o Indicate peaks with a polygon
plot(xchr)

## Add a second peak to the data.
pks <- rbind(chromPeaks(xchr), c(7, 7, 10, NA, 15, NA))
chromPeaks(xchr) <- pks

## Plot the peaks in different colors
plot(xchr, peakCol = c("#ff000080", "#0000ff80"),
    peakBg = c("#ff000020", "#0000ff20"))

## Indicate the peaks as rectangles
plot(xchr, peakCol = c("#ff000060", "#0000ff60"), peakBg = NA,
    peakType = "rectangle")

## Filter the XChromatogram by retention time
xchr_sub <- filterRt(xchr, rt = c(4, 6))
xchr_sub
plot(xchr_sub)
```

---

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.

- `profBin`, `profBinM`, `profBinLin`, `profBinLinM`, `profBinLinBase`, `profBinLinBaseM` have been deprecated and `binYonX` in combination with `imputeLinInterpol` should be used instead.
- `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 matricies with retention time and intensity

`mzrange`: two column matrix containing starting and ending m/z for each EIC

`rtrange`: two column matrix containing starting and ending time for each EIC

`rt`: either `"raw"` or `"corrected"` to specify retention times contained in the object

`groupnames`: group names from `xcmsSet` object used to generate EICs

Methods

groupnames `signature(object = "xcmsEIC")`: get `groupnames` slot

mzrange `signature(object = "xcmsEIC")`: get `mzrange` slot

plot `signature(x = "xcmsEIC")`: plot the extracted ion chromatograms

rtrange `signature(object = "xcmsEIC")`: get `rtrange` slot

sampnames `signature(object = "xcmsEIC")`: get sample names

Note

No notes yet.

Author(s)

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

See Also

getEIC

---

xcmsFileSource-class *Base class for loading raw data from a file*

Description

Data sources which read data from a file should inherit from this class. The xcms package provides classes to read from netCDF, mzData, mzXML, and mzML files using xcmsFileSource.

This class should be considered virtual and will not work if passed to loadRaw-methods. The reason it is not explicitly virtual is that there does not appear to be a way for a class to be both virtual and have a data part (which lets functions treat objects as if they were character strings).

This class validates that a file exists at the path given.

Objects from the Class

xcmsFileSource objects should not be instantiated directly. Instead, create subclasses and instantiate those.

Slots

.Data: Object of class "character". File path of a file from which to read raw data as the object's data part

Extends

Class "character", from data part. Class "xcmsSource", directly.

Methods

xcmsSource signature(object = "character"): Create an xcmsFileSource object referencing the given file name.

Author(s)

Daniel Hackney <dan@haxney.org>

See Also

xcmsSource

`xcmsFragments` *Constructor for xcmsFragments objects which holds Tandem MS peaks*

Description

EXPERIMANTAL FEATURE

xcmsFragments is an object similar to xcmsSet, which holds peaks picked (or collected) from one or several xcmsRaw objects.

There are still discussions going on about the exact API for MS^n data, so this is likely to change in the future. The code is not yet pipeline-ified.

Usage

```
xcmsFragments(xs, ...)
```

Arguments

`xs`	A `xcmsSet-class` object which contains picked ms1-peaks from one or several experiments
`...`	further arguments to the `collect` method

Details

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

Value

An `xcmsFragments` object.

Author(s)

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

See Also

`xcmsFragments-class`, `collect`

`xcmsFragments-class` *Class xcmsFragments, a class for handling Tandem MS and MS^n data*

Description

This class is similar to `xcmsSet` because it stores peaks from a number of individual files. However, xcmsFragments keeps Tandem MS and e.g. Ion Trap or Orbitrap MS^n peaks, including the parent ion relationships.

Objects from the Class

Objects can be created with the `xcmsFragments` constructor and filled with peaks using the collect method.

Slots

`peaks`**:** matrix with colmns peakID (MS1 parent in corresponding xcmsSet), MSnParentPeakID (parent peak within this xcmsFragments), msLevel (e.g. 2 for Tandem MS), rt (retention time in case of LC data), mz (fragment mass-to-charge), intensity (peak intensity extracted from the original `xcmsSet`), sample (the index of the rawData-file).

`MS2spec`**:** This is a list of matrixes. Each matrix in the list is a single collected spectra from `collect`. The column ID's are mz, intensity, and full width half maximum(fwhm). The fwhm column is only relevant if the spectra came from profile data.

`specinfo`**:** This is a matrix with reference data for the spectra in MS2spec. The column id's are preMZ, AccMZ, rtmin, rtmax, ref, CollisionEnergy. The preMZ is precursor mass from the MS1 scan. This mass is given by the XML file. With some instruments this mass is only given as nominal mass, therefore a AccMZ is given which is a weighted average mass from the MS1 scan of the collected spectra. The retention time is given by rtmin and rtmax. The ref column is a pointer to the MS2spec matrix spectra. The collisionEnergy column is the collision Energy for the spectra.

Methods

collect `signature(object = "xcmsFragments")`: gets a xcmsSet-object, collects ms1-peaks from it and the msn-peaks from the corresponding xcmsRaw-files.

plotTree `signature(object = "xcmsFragments")`: prints a (text based) pseudo-tree of the peak-table to display the dependencies of the peaks among each other.

show `signature(object = "xcmsFragments")`: print a human-readable description of this object to the console.

Author(s)

S. Neumann, J. Kutzera

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 data 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 (see further below for specific function to handle chromatographic peak data, alignment and correspondence results):

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 x m matrix, n (rows) representing equally spaced m/z values (bins) and m (columns) the retention time of the corresponding scans. Each cell contains the maximum intensity measured for the specific scan and m/z values. See profMat for more details and description of the various binning methods.

hasAdjustedRtime: whether the object provides adjusted retention times.

hasFeatures: whether the object contains correspondence results (i.e. features).

hasChromPeaks: whether the object contains peak detection results.

hasFilledChromPeaks: whether the object contains any filled-in chromatographic peaks.

adjustedRtime,adjustedRtime<-: extract/set adjusted retention times. adjustedRtime<- should not be called manually, it is called internally by the adjustRtime methods. For XCMSnExp objects, adjustedRtime<- does also apply retention time adjustments to eventually present chromatographic peaks. The bySample parameter allows to specify whether the adjusted retention time should be grouped by sample (file).

featureDefinitions, featureDefinitions<-: extract or set the correspondence results, i.e. the mz-rt features (peak groups). Similar to the chromPeaks it is possible to extract features for specified m/z and/or rt ranges. 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 (i.e. for which either "mzmin" or "mzmax" of the chromPeaks or featureDefinitions matrix are within the provided m/z range), for type == "within" the full peak has to be within the region (i.e. both "mzmin" and "mzmax" have to be within the m/z range) and for type == "apex_within" the peak's apex position (highest signal of the peak) has to be within the region (i.e. the peak's or features m/z has to be within the m/z range). 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. Also, chromPeaks<- will replace any existing chromPeakData.

chromPeakData and chromPeakData<- allow to get or set arbitrary chromatographic peak annotations. These are returned or ar returned as a DataFrame. Note that the number of rows and the rownames of the DataFrame have to match those of chromPeaks.

rtime: extracts the retention time for each scan. The bySample parameter allows to return the values grouped by sample/file and adjusted whether adjusted or raw retention times should be returned. By default the method returns adjusted retention times, if they are available (i.e. if retention times were adjusted using the adjustRtime method).

mz: extracts the mz values from each scan of all files within an XCMSnExp object. These values are extracted from the original data files and eventual processing steps are applied *on the fly*. Using the bySample parameter it is possible to switch from the default grouping of mz values by spectrum/scan to a grouping by sample/file.

intensity: extracts the intensity values from each scan of all files within an XCMSnExp object. These values are extracted from the original data files and eventual processing steps are applied *on the fly*. Using the bySample parameter it is possible to switch from the default grouping of intensity values by spectrum/scan to a grouping by sample/file.

spectra: extracts the Spectrum objects containing all data from object. The values are extracted from the original data files and eventual processing steps are applied *on the fly*. By setting bySample = TRUE, the spectra are returned grouped by sample/file. If the XCMSnExp object contains adjusted retention times, these are returned by default in the Spectrum objects (can be overwritten by setting adjusted = FALSE).

processHistory: returns a list of 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 by default (with parameter add = FALSE) previous peak detection results are removed. Use add = TRUE to perform a second round of peak detection and add the newly identified peaks to the previous peak detection results. Correspondence results (features) are always removed prior to peak detection. 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).

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.

plot plots the spectrum data (see plot for MSnExp objects in the MSnbase package for more details. For type = "XIC", identified chromatographic peaks will be indicated as rectangles with border color peakCol.

Usage

```
processHistoryTypes()

## S4 method for signature 'XCMSnExp'
hasFilledChromPeaks(object)

## S4 method for signature 'OnDiskMSnExp'
profMat(
  object,
  method = "bin",
  step = 0.1,
  baselevel = NULL,
  basespace = NULL,
  mzrange. = NULL,
  fileIndex,
  ...
)
```

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

## S4 method for signature 'XCMSnExp'
hasAdjustedRtime(object)

## S4 method for signature 'XCMSnExp'
hasFeatures(object, msLevel = integer())

## S4 method for signature 'XCMSnExp'
hasChromPeaks(object, msLevel = integer())

## S4 method for signature 'XCMSnExp'
hasFilledChromPeaks(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"),
  msLevel = integer()
)

## S4 replacement method for signature 'XCMSnExp'
featureDefinitions(object) <- value

## S4 method for signature 'XCMSnExp'
chromPeaks(
  object,
  bySample = FALSE,
  rt = numeric(),
  mz = numeric(),
  ppm = 0,
  msLevel = integer(),
  type = c("any", "within", "apex_within"),
  isFilledColumn = FALSE
)

## 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,
  add = FALSE
)

## S4 method for signature 'XCMSnExp'
dropFilledChromPeaks(object)

## S4 method for signature 'XCMSnExp'
spectrapply(object, FUN = NULL, BPPARAM = bpparam(), ...)

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

## S4 method for signature 'XCMSnExp'
chromPeakData(object, ...)

## S4 replacement method for signature 'XCMSnExp'
chromPeakData(object) <- value

## S4 method for signature 'XCMSnExp,missing'
plot(x, y, type = c("spectra", "XIC"), peakCol = "#ff000060", ...)
```

Arguments

object	For adjustedRtime, featureDefinitions, chromPeaks, hasAdjustedRtime, hasFeatures and hasChromPeaks either a MsFeatureData or a XCMSnExp object, for all other methods a XCMSnExp object.
method	character(1) defining 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 binnind. If not provided, the whole m/z value range is used.
fileIndex	For processHistory: optional integer specifying the index of the files/samples for which the ProcessHistory objects should be retrieved.
...	Additional parameters.

msLevel — integer specifying the MS level(s) for which identified chromatographic peaks should be returned.

bySample — logical(1) specifying whether results should be grouped by sample.

value — For adjustedRtime<-: a list (length equal to the number of samples) with numeric vectors representing the adjusted retention times per scan.

For featureDefinitions<-: a DataFrame with peak grouping information. See return value for the featureDefinitions method for the expected format.

For chromPeaks<-: a matrix with information on detected peaks. See return value for the chromPeaks method for the expected format.

mz — optional numeric(2) defining the mz range for which chromatographic peaks should be returned.

rt — optional numeric(2) defining the retention time range for which chromatographic peaks should be returned.

ppm — optional numeric(1) specifying the ppm by which the mz range should be extended. For a value of ppm = 10, all peaks within mz[1] - ppm / 1e6 and mz[2] + ppm / 1e6 are returned.

type — For processHistory: restrict returned ProcessHistory objects to analysis steps of a certain type. Use the processHistoryTypes to list all supported values. For chromPeaks: character specifying which peaks to return if rt or mz are defined. For type = "any" all chromatographic peaks 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.

isFilledColumn — logical(1) whether a column "is_filled" is included in the returned "matrix" providing the information if a peak was filled in. Alternatively, this information would be provided by the chromPeakData data frame.

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.

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".

add	For findChromPeaks: if newly identified chromatographic peaks should be added to the peak matrix with the already identified chromatographic peaks. By default (add = FALSE) previous peak detection results will be removed.
FUN	For spectrapply: a function that should be applied to each spectrum in the object.
x	For plot: XCMSnExp object.
y	For plot: not used.
peakCol	For plot: the color that should be used to indicate identified chromatographic peaks (only in combination with type = "XIC" and if chromatographic peaks are present).

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. featureDefinitions supports also parameters mz, rt, ppm and type to return only features within certain ranges (see description of chromPeaks for details).

For chromPeaks: if bySample = FALSE a matrix (each row being a chromatographic peak, rownames 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 of the peak apex), "rtmin" (minimal retention time), "rtmax" (maximal retention time), "into" (integrated, original, intensity of the peak), "maxo" (maximum intentity of the peak), "sample" (sample index in which the peak was identified) and Depending on the employed peak detection algorithm and the verboseColumns parameter of it, additional columns might be returned. If parameter isFilledColumn was set to TRUE a column named "is_filled" is also 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).
- overlappingFeatures identify features that are overlapping or close in the m/z - rt space (see respective help page).
- quantify extract feature intensities and put them, along with feature definitions and phenodata information, into a SummarizedExperiment. See help page for details.

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

```
## Load a test data set with detected peaks
library(MSnbase)
data(faahko_sub)
## Update the path to the files for the local system
dirname(faahko_sub) <- system.file("cdf/KO", package = "faahKO")

## Disable parallel processing for this example
register(SerialParam())

## The results from the peak detection are now stored in the XCMSnExp
## object
faahko_sub

## The detected peaks can be accessed with the chromPeaks method.
head(chromPeaks(faahko_sub))

## The settings of the chromatographic peak detection can be accessed with
## the processHistory method
processHistory(faahko_sub)

## Also the parameter class for the peak detection can be accessed
processParam(processHistory(faahko_sub)[[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(faahko_sub))

## 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(faahko_sub, 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(faahko_sub)
## To get all spectra of the first file we can split them by file
## head(split(spctr, fromFile(faahko_sub))[[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(faahko_sub, file = 2)
xod_2

## Now the objects contains only the idenfified peaks for the second file
head(chromPeaks(xod_2))

##########
## Coercing to an xcmsSet object
##
## We can also coerce the XCMSnExp object into an xcmsSet object:
xs <- as(faahko_sub, "xcmsSet")
head(peaks(xs))
```

`xcmsPeaks-class` *A matrix of peaks*

Description

A matrix of peak information. The actual columns depend on how it is generated (i.e. the `findPeaks` method).

Objects from the Class

Objects can be created by calls of the form `new("xcmsPeaks", ...)`.

Slots

`.Data`: The matrix holding the peak information

Extends

Class `"matrix"`, from data part. Class `"array"`, by class "matrix", distance 2. Class `"structure"`, by class "matrix", distance 3. Class `"vector"`, by class "matrix", distance 4, with explicit coerce.

Methods

None yet. Some utilities for working with peak data would be nice.

Author(s)

Michael Lawrence

See Also

`findPeaks` for detecting peaks in an `xcmsRaw`.

xcmsRaw *Constructor for xcmsRaw objects which reads NetCDF/mzXML files*

Description

This function handles the task of reading a NetCDF/mzXML file containing LC/MS or GC/MS data into a new xcmsRaw object. It also transforms the data into profile (maxrix) mode for efficient plotting and data exploration.

Usage

```
xcmsRaw(filename, profstep = 1, profmethod = "bin", profparam =
list(), includeMSn=FALSE, mslevel=NULL, scanrange=NULL)

deepCopy(object)
```

Arguments

filename	path name of the NetCDF or mzXML file to read
profstep	step size (in m/z) to use for profile generation
profmethod	method to use for profile generation. See profile-matrix for details and supported values.
profparam	extra parameters to use for profile generation
includeMSn	only for XML file formats: also read MS^n (Tandem-MS of Ion-/Orbi- Trap spectra)
mslevel	move data from mslevel into normal MS1 slots, e.g. for peak picking and visualisation
scanrange	scan range to read
object	An xcmsRaw object

Details

See profile-matrix for details on profile matrix generation methods and settings.

The scanrange to import can be restricted, otherwise all MS1 data is read. If profstep is set to 0, no profile matrix is generated. Unless includeMSn = TRUE only first level MS data is read, not MS/MS, etc.

deepCopy(xraw) will create a copy of the xcmsRaw object with its own copy of mz and intensity data in xraw@env.

Value

A xcmsRaw object.

Author(s)

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

References

NetCDF file format: https://www.unidata.ucar.edu/software/netcdf/ http://www.astm.org/Standards/E2077.htm http://www.astm.org/Standards/E2078.htm

mzXML file format: http://sashimi.sourceforge.net/software_glossolalia.html

PSI-MS working group who developed mzData and mzML file formats: http://www.psidev.info/index.php?q=node/80

Parser used for XML file formats: http://tools.proteomecenter.org/wiki/index.php?title=Software:RAMP

See Also

xcmsRaw-class, profStep, profMethod xcmsFragments

Examples

```
## Not run:
    library(xcms)
    library(faahKO)
    cdfpath <- system.file("cdf", package = "faahKO")
    cdffiles <- list.files(cdfpath, recursive = TRUE, full.names = TRUE)
    xr<-xcmsRaw(cdffiles[1])
    xr
    ##This gives some information about the file
    names(attributes(xr))
    ## Lets have a look at the structure of the object

    str(xr)
    ##same but with a preview of each slot in the object
    ##SO... lets have a look at how this works
    head(xr@scanindex)
    ##[1]    0  429  860 1291 1718 2140
    xr@env$mz[425:430]
    ##[1] 596.3 597.0 597.3 598.1 599.3 200.1
    ##We can see that the 429 index is the last mz of scan 1 therefore...

    mz.scan1<-xr@env$mz[(1+xr@scanindex[1]):xr@scanindex[2]]
    intensity.scan1<-xr@env$intensity[(1+xr@scanindex[1]):xr@scanindex[2]]
    plot(mz.scan1, intensity.scan1, type="h",
         main=paste("Scan 1 of file", basename(cdffiles[1]), sep=""))
    ##the easier way :p
    scan1<-getScan(xr, 1)
    head(scan1)
    plotScan(xr, 1)

## End(Not run)
```

xcmsRaw-class *Class xcmsRaw, a class for handling raw data*

Description

This class handles processing and visualization of the raw data from a single LC/MS or GS/MS run. It includes methods for producing a standard suite of plots including individual spectra, multi-scan average spectra, TIC, and EIC. It will also produce a feature list of significant peaks using matched filtration.

Objects from the Class

Objects can be created with the `xcmsRaw` constructor which reads data from a NetCDF file into a new object.

Slots

`acquisitionNum`: Numeric representing the acquisition number of the individual scans/spectra. Length of `acquisitionNum` is equal to the number of spectra/scans in the object and hence equal to the `scantime` slot. Note however that this information is only available in mzML files.

`env`: environment with three variables: `mz` - concatenated m/z values for all scans, `intensity` - corresponding signal intensity for each m/z value, and `profile` - matrix represention of the intensity values with columns representing scans and rows representing equally spaced m/z values. The profile matrix should be extracted with the `profMat` method.

`filepath`: Path to the raw data file

`gradient`: matrix with first row, `time`, containing the time point for interpolation and successive columns representing solvent fractions at each point

`msnAcquisitionNum`: for each scan a unique acquisition number as reported via "spectrum id" (mzData) or "<scan num=...>" and "<scanOrigin num=...>" (mzXML)

`msnCollisionEnergy`: "CollisionEnergy" (mzData) or "collisionEnergy" (mzXML)

`msnLevel`: for each scan the "msLevel" (both mzData and mzXML)

`msnPrecursorCharge`: "ChargeState" (mzData) and "precursorCharge" (mzXML)

`msnPrecursorIntensity`: "Intensity" (mzData) or "precursorIntensity" (mzXML)

`msnPrecursorMz`: "MassToChargeRatio" (mzData) or "precursorMz" (mzXML)

`msnPrecursorScan`: "spectrumRef" (both mzData and mzXML)

`msnRt`: Retention time of the scan

`msnScanindex`: msnScanindex

`mzrange`: numeric vector of length 2 with minimum and maximum m/z values represented in the profile matrix

`polarity`: polarity

`profmethod`: characer value with name of method used for generating the profile matrix.

`profparam`: list to store additional profile matrix generation settings. Use the `profinfo` method to extract all profile matrix creation relevant information.

`scanindex`: integer vector with starting positions of each scan in the `mz` and `intensity` variables (note that index values are based off a 0 initial position instead of 1).

`scantime`: numeric vector with acquisition time (in seconds) for each scan.

`tic`: numeric vector with total ion count (intensity) for each scan

`mslevel`: Numeric representing the MS level that is present in MS1 slot. This slot should be accessed through its getter method `mslevel`.

`scanrange`: Numeric of length 2 specifying the scan range (or `NULL` for the full range). This slot should be accessed through its getter method `scanrange`. Note that the `scanrange` will always be 1 to the number of scans within the `xcmsRaw` object, which does not necessarily have to match to the scan index in the original mzML file (e.g. if the original data was subsetted). The `acquisitionNum` information can be used to track the original *position* of each scan in the mzML file.

Methods

findPeaks `signature(object = "xcmsRaw")`: feature detection using matched filtration in the chromatographic time domain

getEIC `signature(object = "xcmsRaw")`: get extracted ion chromatograms in specified m/z ranges. This will return the total ion chromatogram (TIC) if the m/z range corresponds to the full m/z range (i.e. sum of all signals per retention time across all m/z).

getPeaks `signature(object = "xcmsRaw")`: get data for peaks in specified m/z and time ranges

getScan `signature(object = "xcmsRaw")`: get m/z and intensity values for a single mass scan

getSpec `signature(object = "xcmsRaw")`: get average m/z and intensity values for multiple mass scans

image `signature(x = "xcmsRaw")`: get data for peaks in specified m/z and time ranges

levelplot Create an image of the raw (profile) data m/z against retention time, with the intensity color coded.

mslevel Getter method for the `mslevel` slot.

plotChrom `signature(object = "xcmsRaw")`: plot a chromatogram from profile data

plotRaw `signature(object = "xcmsRaw")`: plot locations of raw intensity data points

plotScan `signature(object = "xcmsRaw")`: plot a mass spectrum of an individual scan from the raw data

plotSpec `signature(object = "xcmsRaw")`: plot a mass spectrum from profile data

plotSurf `signature(object = "xcmsRaw")`: experimental method for plotting 3D surface of profile data with `rgl`.

plotTIC `signature(object = "xcmsRaw")`: plot total ion count chromatogram

profinfo `signature(object = "xcmsRaw")`: returns a list containing the profile generation method and step (profile m/z step size) and eventual additional parameters to the profile function.

profMedFilt `signature(object = "xcmsRaw")`: median filter profile data in time and m/z dimensions

profMethod<- `signature(object = "xcmsRaw")`: change the method of generating the `profile` matrix

profMethod `signature(object = "xcmsRaw")`: get the method of generating the `profile` matrix

profMz `signature(object = "xcmsRaw")`: get vector of m/z values for each row of the `profile` matrix

profRange `signature(object = "xcmsRaw")`: interpret flexible ways of specifying subsets of the `profile` matrix

profStep<- `signature(object = "xcmsRaw")`: change the m/z step used for generating the `profile` matrix

profStep `signature(object = "xcmsRaw")`: get the m/z step used for generating the `profile` matrix

revMz `signature(object = "xcmsRaw")`: reverse the order of the data points for each scan

scanrange Getter method for the `scanrange` slot. See slot description above for more information.

sortMz `signature(object = "xcmsRaw")`: sort the data points by increasing m/z for each scan

stitch `signature(object = "xcmsRaw")`: Raw data correction for lock mass calibration gaps.

findmzROI `signature(object = "xcmsRaw")`: internal function to identify regions of interest in the raw data as part of the first step of centWave-based peak detection.

Author(s)

Colin A. Smith, <csmith@scripps.edu>, Johannes Rainer <johannes.rainer@eurac.edu>

See Also

xcmsRaw, subset-xcmsRaw for subsetting by spectra.

`xcmsSet` *Constructor for xcmsSet objects which finds peaks in NetCDF/mzXML files*

Description

This function handles the construction of xcmsSet objects. It finds peaks in batch mode and pre-sorts files from subdirectories into different classes suitable for grouping.

Usage

```
xcmsSet(files = NULL, snames = NULL, sclass = NULL, phenoData = NULL,
        profmethod = "bin", profparam = list(),
        polarity = NULL, lockMassFreq=FALSE,
mslevel=NULL, nSlaves=0, progressCallback=NULL,
        scanrange = NULL, BPPARAM = bpparam(),
        stopOnError = TRUE, ...)
```

Arguments

files	path names of the NetCDF/mzXML files to read
snames	sample names. By default the file name without extension is used.
sclass	sample classes.
phenoData	data.frame or AnnotatedDataFrame defining the sample names and classes and other sample related properties. If not provided, the argument sclass or the subdirectories in which the samples are stored will be used to specify sample grouping.
profmethod	Method to use for profile generation. Supported values are "bin", "binlin", "binlinbase" and "intlin" (for methods profBin, profBinLin, profBinLinBase and profIntLin, respectively). See help on profBin for a complete list of available methods and their supported parameters.
profparam	parameters to use for profile generation.
polarity	filter raw data for positive/negative scans
lockMassFreq	Performs correction for Waters LockMass function
mslevel	perform peak picking on data of given mslevel
nSlaves	*DEPRECATED*, use BPPARAM argument instead.
progressCallback	function to be called, when progressInfo changes (useful for GUIs)
scanrange	scan range to read
BPPARAM	a BiocParallel parameter object to control how and if parallel processing should be performed. Such objects can be created by the SerialParam, MulticoreParam or SnowParam functions.
stopOnError	Logical specifying whether the feature detection call should stop on the first encountered error (the default), or whether feature detection is performed in all files regardless eventual failures for individual files in which case all errors are reported as warnings.
...	further arguments to the findPeaks method of the xcmsRaw class

Details

The default values of the files, snames, sclass, and phenoData arguments cause the function to recursively search for readable files. The filename without extention is used for the sample name. The subdirectory path is used for the sample class. If the files contain both positive and negative spectra, the polarity can be selected explicitly. The default (NULL) is to read all scans.

If phenoData is provided, it is stored to the phenoData slot of the returned xcmsSet class. If that data.frame contains a column named "class", its content will be returned by the sampclass method and thus be used for the group/class assignment of the individual files (e.g. for peak grouping etc.). For more details see the help of the xcmsSet-class.

The step size (in m/z) to use for profile generation can be submitted either using the profparam argument (e.g. profparam=list(step=0.1)) or by submitting step=0.1. By specifying a value of 0 the profile matrix generation can be skipped.

The feature/peak detection algorithm can be specified with the method argument which defaults to the "matchFilter" method (findPeaks.matchedFilter). Possible values are returned by getOption("BioC")$xcms$findPeaks.methods.

The lock mass correction allows for the lock mass scan to be added back in with the last working scan. This correction gives better reproducibility between sample sets.

Value

A xcmsSet object.

Note

The arguments profmethod and profparam have no influence on the feature/peak detection. The step size parameter step for the profile generation in the findPeaks.matchedFilter peak detection algorithm can be passed using the ....

Author(s)

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

See Also

xcmsSet-class, findPeaks, profStep, profMethod, profBin

---

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 = profStep(object), profparam=profinfo(object), mslevel = NULL, scanrange = NULL, rt=c("corrected", "raw"), BPPARAM = bpparam())`: 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`).

Author(s)

Colin A. Smith, <csmith@scripps.edu>, Johannes Rainer <johannes.rainer@eurac.edu>

See Also

`xcmsSet`

`xcmsSource-class` *Virtual class for raw data sources*

Description

This virtual class provides an implementation-independent way to load mass spectrometer data from various sources for use in an `xcmsRaw` object. Subclasses can be defined to enable data to be loaded from user-specified sources. The virtual class `xcmsFileSource` is included out of the box which contains a file name as a character string.

When implementing child classes of `xcmsSource`, a corresponding `loadRaw-methods` method must be provided which accepts the `xcmsSource` child class and returns a list in the format described in `loadRaw-methods`.

Objects from the Class

A virtual Class: No objects may be created from it.

Author(s)

Daniel Hackney, <dan@haxney.org>

See Also

`xcmsSource-methods` for creating `xcmsSource` objects in various ways.

xcmsSource-methods *Create an xcmsSource object in a flexible way*

Description

Users can define alternate means of reading data for xcmsRaw objects by creating new implementations of this method.

Methods

`signature(object = "xcmsSource")` Pass the object through unmodified.

Author(s)

Daniel Hackney, <dan@haxney.org>

See Also

xcmsSource

[,XCMSnExp,ANY,ANY,ANY-method *XCMSnExp filtering and subsetting*

Description

The methods listed on this page allow to filter and subset XCMSnExp objects. Most of them are inherited from the OnDiskMSnExp object defined in the MSnbase package and have been adapted for XCMSnExp to enable correct subsetting of preprocessing results.

- `[`: subset a XCMSnExp object by spectra. Be aware that this removes **all** preprocessing results, except adjusted retention times if `keepAdjustedRtime = TRUE` is passed to the method.
- `[[`: extracts a single Spectrum object (defined in MSnbase). The reported retention time is the adjusted retention time if alignment has been performed.
- `filterChromPeaks`: subset the `chromPeaks` matrix in `object`. Parameter `method` allows to specify how the chromatographic peaks should be filtered. Currently, only `method = "keep"` is supported which allows to specify chromatographic peaks to keep with parameter `keep` (i.e. provide a `logical`, `integer` or `character` defining which chromatographic peaks to keep). Feature definitions (if present) are updated correspondingly.
- `filterFeatureDefinitions`: allows to subset the feature definitions of an XCMSnExp object. Parameter `features` allow to define which features to keep. It can be a `logical`, `integer` (index of features to keep) or `character` (feature IDs) vector.

- `filterFile`: allows to reduce the `XCMSnExp` to data from only selected files. Identified chromatographic peaks for these files are retained while correspondence results (feature definitions) are removed by default. To force keeping feature definitions use `keepFeatures = TRUE`. Adjusted retention times (if present) are retained by default if present. Use `keepAdjustedRtime = FALSE` to drop them.
- `filterMsLevel`: reduces the `XCMSnExp` object to spectra of the specified MS level(s). Chromatographic peaks and identified features are also subsetted to the respective MS level. See also the `filterMsLevel` documentation in `MSnbase` for details and examples.
- `filterMz`: filters the data set based on the provided m/z value range. All chromatographic peaks and features (grouped peaks) with their apex falling within the provided mz value range are retained (i.e. if `chromPeaks(object)[, "mz"]` is `>= mz[1]` and `<= mz[2]`). Adjusted retention times, if present, are kept.
- `filterRt`: filters the data set based on the provided retention time range. All chromatographic peaks and features (grouped peaks) within 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 on raw or adjusted retention times. Filtering by retention time does not drop any preprocessing results nor does it remove or change alignment results (i.e. adjusted retention times). The method returns an empty object if no spectrum or feature is within the specified retention time range.
- `split`: splits an `XCMSnExp` object into a `list` of `XCMSnExp` objects based on the provided parameter `f`. Note that by default all pre-processing results are removed by the splitting, except adjusted retention times, if the optional argument `keepAdjustedRtime = TRUE` is provided.

Usage

```
## S4 method for signature 'XCMSnExp,ANY,ANY,ANY'
x[i, j, ..., drop = TRUE]

## S4 method for signature 'XCMSnExp,ANY,ANY'
x[[i, j, drop = FALSE]]

## S4 method for signature 'XCMSnExp'
filterMsLevel(object, msLevel., keepAdjustedRtime = hasAdjustedRtime(object))

## S4 method for signature 'XCMSnExp'
filterFile(
  object,
  file,
  keepAdjustedRtime = hasAdjustedRtime(object),
  keepFeatures = 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, ...)

## S4 method for signature 'XCMSnExp'
filterChromPeaks(
  object,
  keep = rep(TRUE, nrow(chromPeaks(object))),
  method = "keep",
  ...
)

## S4 method for signature 'XCMSnExp'
filterFeatureDefinitions(object, features = integer())
```

Arguments

x	For [and [[: an XCMSnExp object.
i	For [: numeric or logical vector specifying to which spectra the data set should be reduced. For [[: a single integer or character.
j	For [and [[: not supported.
...	Optional additional arguments.
drop	For [and [[: not supported.
object	A XCMSnExp object.
msLevel.	For filterMz, filterRt: numeric defining the MS level(s) to which operations should be applied or to which the object should be subsetted.
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.
keepFeatures	For filterFile: logical(1) whether correspondence results (feature definitions) should be kept or dropped. Defaults to keepFeatures = FALSE hence feature definitions are removed from the returned object by default.
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 should be splitted. It is converted internally to a factor.
keep	For filterChromPeaks: logical, integer or character defining which chromatographic peaks should be retained.
method	For filterChromPeaks: character(1) allowing to specify the method by which chromatographic peaks should be filtered. Currently only method = "keep" is supported (i.e. specify with parameter keep which chromatographic peaks should be retained).
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.

Details

All subsetting methods try to ensure that the returned data is consistent. Correspondence results for example are removed by default if the data set is sub-setted by file, since the correspondence results are dependent on the files on which correspondence was performed. This can be changed by setting keepFeatures = TRUE. For 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.

XChromatograms() for similar filter functions on XChromatograms objects.

Examples

```
## Loading a test data set with identified chromatographic peaks
library(MSnbase)
data(faahko_sub)
## Update the path to the files for the local system
dirname(faahko_sub) <- system.file("cdf/KO", package = "faahKO")

## Disable parallel processing for this example
register(SerialParam())

## Subset the dataset to the first and third file.
xod_sub <- filterFile(faahko_sub, file = c(1, 3))

## The number of chromatographic peaks per file for the full object
table(chromPeaks(faahko_sub)[, "sample"])

## The number of chromatographic peaks per file for the subset
table(chromPeaks(xod_sub)[, "sample"])

basename(fileNames(faahko_sub))
basename(fileNames(xod_sub))

## Filter on mz values; chromatographic peaks and features within the
## mz range are retained (as well as adjusted retention times).
xod_sub <- filterMz(faahko_sub, mz = c(300, 400))
head(chromPeaks(xod_sub))
nrow(chromPeaks(xod_sub))
nrow(chromPeaks(faahko_sub))

## 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(faahko_sub, rt = c(2700, 2900))

range(rtime(xod_sub))
head(chromPeaks(xod_sub))
range(chromPeaks(xod_sub)[, "rt"])

nrow(chromPeaks(faahko_sub))
nrow(chromPeaks(xod_sub))

## Extract a single Spectrum
faahko_sub[[4]]

## Subsetting using [ removes all preprocessing results - using
## keepAdjustedRtime = TRUE would keep adjusted retention times, if present.
xod_sub <- faahko_sub[fromFile(faahko_sub) == 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(faahko_sub, f = fromFile(faahko_sub))
xod_list
```

`[,xcmsRaw,logicalOrNumeric,missing,missing-method`
Subset an xcmsRaw object by scans

Description

Subset an `xcmsRaw` object by scans. The returned `xcmsRaw` object contains values for all scans specified with argument `i`. Note that the `scanrange` slot of the returned `xcmsRaw` will be `c(1, length(object@scantime))` and hence not `range(i)`.

Usage

```
## S4 method for signature 'xcmsRaw,logicalOrNumeric,missing,missing'
x[i, j, drop]
```

Arguments

`x`	The `xcmsRaw` object that should be sub-setted.
`i`	Integer or logical vector specifying the scans/spectra to which `x` should be sub-setted.
`j`	Not supported.
`drop`	Not supported.

Details

Only subsetting by scan index in increasing order or by a logical vector are supported. If not ordered, argument `i` is sorted automatically. Indices which are larger than the total number of scans are discarded.

Value

The sub-setted `xcmsRaw` object.

Author(s)

Johannes Rainer

See Also

`split.xcmsRaw`

Examples

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

Index

∗ **Filter features in xcms**
BlankFlag, 26
DratioFilter, 75
PercentMissingFilter, 218
RsdFilter, 269
∗ **NA**
na.flatfill, 210
∗ **aplot**
panel.cor, 211
∗ **array**
colMax, 43
rectUnique, 258
∗ **chromatographic peak refinement methods**
refineChromPeaks, 259
∗ **classes**
xcmsEIC-class, 301
xcmsFileSource-class, 302
xcmsFragments-class, 304
xcmsPeaks-class, 316
xcmsRaw-class, 319
xcmsSet-class, 323
xcmsSource-class, 326
∗ **core peak detection functions**
do_findChromPeaks_centWave, 52
do_findChromPeaks_centWaveWithPredIsoROIs, 56
do_findChromPeaks_massifquant, 61
do_findChromPeaks_matchedFilter, 64
do_findPeaks_MSW, 67
∗ **core peak grouping algorithms**
do_groupChromPeaks_density, 69
do_groupChromPeaks_nearest, 72
do_groupPeaks_mzClust, 73
∗ **core retention time correction algorithms**
do_adjustRtime_peakGroups, 50
∗ **feature grouping methods**
groupFeatures-abundance-correlation, 186
groupFeatures-eic-similarity, 187
groupFeatures-similar-rtime, 191
∗ **file**
calibrate-methods, 33
diffreport-methods, 47
fillPeaks-methods, 94
fillPeaks.chrom-methods, 95
fillPeaks.MSW-methods, 96
getEIC-methods, 172
getXcmsRaw-methods, 175
group.density, 177
group.mzClust, 178
group.nearest, 179
groupnames-methods, 193
peakTable-methods, 217
retcor.peakgroups-methods, 267
sampnames-methods, 271
verify.mzQuantM, 283
write.cdf-methods, 284
write.mzdata-methods, 285
write.mzQuantML-methods, 285
writeMzTab, 287
xcmsFileSource-class, 302
xcmsFragments, 303
xcmsRaw, 317
xcmsSet, 321
∗ **functions to define bins**
breaks_on_binSize, 28
breaks_on_nBins, 29
∗ **hplot**
image-methods, 197
levelplot-methods, 203
plot.xcmsEIC, 222
plotChrom-methods, 225
plotPeaks-methods, 236
plotRaw-methods, 238
plotrt-methods, 238
plotScan-methods, 239

plotSpec-methods, 240
plotSurf-methods, 240
plotTIC-methods, 241
∗ **imputation functions**
imputeRowMin, 199
imputeRowMinRand, 200
∗ **internal**
colMax, 43
descendZero, 46
doubleMatrix, 49
filtfft, 117
findEqualGreater, 147
na.flatfill, 210
panel.cor, 211
profGenerate, 243
pval, 251
rectUnique, 258
∗ **iplot**
plotChrom-methods, 225
plotSpec-methods, 240
plotSurf-methods, 240
plotTIC-methods, 241
∗ **iteration**
descendZero, 46
∗ **lockmass**
AutoLockMass-methods, 20
∗ **manip**
AutoLockMass-methods, 20
c-methods, 30
colMax, 43
getPeaks-methods, 173
getScan-methods, 174
getSpec-methods, 174
groupval-methods, 194
medianFilter, 208
msn2xcmsRaw, 209
profGenerate, 243
profMedFilt-methods, 248
profMethod-methods, 248
profRange-methods, 249
profStep-methods, 250
retexp, 268
specNoise, 275
specPeaks, 276
split.xcmsRaw, 277
split.xcmsSet, 278
stitch-methods, 279
∗ **math**
filtfft, 117
∗ **methods**
absent-methods, 7
AutoLockMass-methods, 20
calibrate-methods, 33
collect-methods, 42
diffreport-methods, 47
fillPeaks-methods, 94
fillPeaks.chrom-methods, 95
fillPeaks.MSW-methods, 96
findMZ, 148
findneutral, 149
findPeaks-methods, 151
findPeaks.addPredictedIsotopeFeatures-methods, 156
findPeaks.centWave-methods, 159
findPeaks.centWaveWithPredictedIsotopeROIs-methods, 161
findPeaks.massifquant-methods, 164
findPeaks.MS1-methods, 168
getEIC-methods, 172
getPeaks-methods, 173
getScan-methods, 174
getSpec-methods, 174
getXcmsRaw-methods, 175
group-methods, 176
group.density, 177
group.mzClust, 178
group.nearest, 179
groupnames-methods, 193
groupval-methods, 194
loadRaw-methods, 203
peakPlots-methods, 212
peakTable-methods, 217
plot.xcmsEIC, 222
plotChrom-methods, 225
plotEIC-methods, 233
plotPeaks-methods, 236
plotRaw-methods, 238
plotrt-methods, 238
plotScan-methods, 239
plotSpec-methods, 240
plotSurf-methods, 240
plotTIC-methods, 241
profMedFilt-methods, 248
profMethod-methods, 248
profRange-methods, 249
profStep-methods, 250

rawEIC-methods, 253
rawMat-methods, 254
retcor-methods, 265
retcor.obiwarp, 266
retcor.peakgroups-methods, 267
sampnames-methods, 271
specDist-methods, 272
specDist.cosine, 273
specDist.meanMZmatch, 274
specDist.peakCount-methods, 275
stitch-methods, 279
write.cdf-methods, 284
write.mzdata-methods, 285
write.mzQuantML-methods, 285
xcmsSource-methods, 327
∗ **models**
etg, 77
∗ **nonlinear**
SSgauss, 278
∗ **peak detection functions for chromatographic data**
peaksWithCentWave, 213
peaksWithMatchedFilter, 215
∗ **peak detection methods**
findChromPeaks, 117
findChromPeaks-centWave, 122
findChromPeaks-centWaveWithPredIsoROIs, 128
findChromPeaks-massifquant, 133
findChromPeaks-matchedFilter, 140
findPeaks-MSW, 152
∗ **peak grouping methods**
groupChromPeaks, 180
∗ **programming**
doubleMatrix, 49
∗ **retention time correction methods**
adjustRtime, 7
∗ **univar**
pval, 251
∗ **utilities**
findEqualGreater, 147
∗ **xcms result export formats.**
PlainTextParam, 220
RDataParam, 255
[,XCMSnExp,ANY,ANY,ANY-method, 327
[,XChromatograms,ANY,ANY,ANY-method *(XChromatograms)*, 288
[,XcmsExperiment,ANY,ANY,ANY-method *(filterFeatureDefinitions)*, 99
[,xcmsRaw,logicalOrNumeric,missing,missing-method, 332
[,xcmsSet,ANY,ANY,ANY-method *(xcmsSet-class)*, 323
[,xcmsSet-method *(xcmsSet-class)*, 323
[[,XCMSnExp,ANY,ANY-method *([,XCMSnExp,ANY,ANY,ANY-method)*, 327
$,xcmsSet-method *(xcmsSet-class)*, 323
$<-,xcmsSet-method *(xcmsSet-class)*, 323

absent *(absent-methods)*, 7
absent,xcmsSet-method *(absent-methods)*, 7
absent-methods, 7
absMz *(groupChromPeaks)*, 180
absMz,MzClustParam-method *(groupChromPeaks)*, 180
absMz,NearestPeaksParam-method *(groupChromPeaks)*, 180
absMz<- *(groupChromPeaks)*, 180
absMz<-,MzClustParam-method *(groupChromPeaks)*, 180
absMz<-,NearestPeaksParam-method *(groupChromPeaks)*, 180
absRt *(groupChromPeaks)*, 180
absRt,NearestPeaksParam-method *(groupChromPeaks)*, 180
absRt<- *(groupChromPeaks)*, 180
absRt<-,NearestPeaksParam-method *(groupChromPeaks)*, 180
AbundanceSimilarityParam(), *81*, *186*
addParams *(findPeaks-MSW)*, 152
addParams,MSWParam-method *(findPeaks-MSW)*, 152
addParams<- *(findPeaks-MSW)*, 152
addParams<-,MSWParam-method *(findPeaks-MSW)*, 152
adjustedRtime *(XCMSnExp-class)*, 305
adjustedRtime,MsFeatureData-method *(XCMSnExp-class)*, 305
adjustedRtime,XcmsExperiment-method *(filterFeatureDefinitions)*, 99
adjustedRtime,XCMSnExp-method *(XCMSnExp-class)*, 305
adjustedRtime<- *(XCMSnExp-class)*, 305
adjustedRtime<-,MsFeatureData-method *(XCMSnExp-class)*, 305

adjustedRtime<-,XCMSnExp-method (XCMSnExp-class), 305
adjustRtime, 7, 305–307, 313, 314
adjustRtime(), 19, 100, 110
adjustRtime,MsExperiment,ObiwarpParam-method (adjustRtime), 7
adjustRtime,MsExperiment,PeakGroupsParam-method (adjustRtime), 7
adjustRtime,OnDiskMSnExp,ObiwarpParam-method (adjustRtime), 7
adjustRtime,XcmsExperiment,LamaParama-method, 15
adjustRtime,XCMSnExp,ObiwarpParam-method (adjustRtime), 7
adjustRtime,XCMSnExp,PeakGroupsParam-method (adjustRtime), 7
adjustRtimePeakGroups (adjustRtime), 7
alignRt(), 188, 189
ampTh (findPeaks-MSW), 152
ampTh,MSWParam-method (findPeaks-MSW), 152
ampTh<- (findPeaks-MSW), 152
ampTh<-,MSWParam-method (findPeaks-MSW), 152
applyAdjustedRtime, 18, 313
applyAdjustedRtime(), 7, 79, 110, 330
array, 316
as, 314
as.list,CentWaveParam-method (findChromPeaks-centWave), 122
as.list,PeakDensityParam-method (groupChromPeaks), 180
AutoLockMass (AutoLockMass-methods), 20
AutoLockMass,xcmsRaw-method (AutoLockMass-methods), 20
AutoLockMass-methods, 20

baseValue (findChromPeaks-matchedFilter), 140
baseValue,MatchedFilterParam-method (findChromPeaks-matchedFilter), 140
baseValue<- (findChromPeaks-matchedFilter), 140
baseValue<-,MatchedFilterParam-method (findChromPeaks-matchedFilter), 140
bin, 21
bin,XCMSnExp-method, 21
binSize (findChromPeaks-matchedFilter), 140
binSize,MatchedFilterParam-method (findChromPeaks-matchedFilter), 140
binSize,ObiwarpParam-method (adjustRtime), 7
binSize,PeakDensityParam-method (groupChromPeaks), 180
binSize<- (findChromPeaks-matchedFilter), 140
binSize<-,MatchedFilterParam-method (findChromPeaks-matchedFilter), 140
binSize<-,ObiwarpParam-method (adjustRtime), 7
binSize<-,PeakDensityParam-method (groupChromPeaks), 180
binYonX, 23, 29, 30, 66, 67, 144, 245, 301
BlankFlag, 26, 27, 76, 115, 219, 270, 271
bpparam, 95, 126, 132, 138, 143, 155, 311
bpparam(), 12, 40, 77, 84, 105, 118, 120, 146, 207, 247, 257, 261
breaks_on_binSize, 25, 28, 30
breaks_on_nBins, 25, 29, 29
bw (groupChromPeaks), 180
bw,PeakDensityParam-method (groupChromPeaks), 180
bw<- (groupChromPeaks), 180
bw<-,PeakDensityParam-method (groupChromPeaks), 180

c, 324
c, c-methods (c-methods), 30
c-methods, 30
c.XCMSnExp (XCMSnExp-class), 305
c.xcmsSet (c-methods), 30
CalibrantMassParam (CalibrantMassParam-class), 31
CalibrantMassParam-class, 31
calibrate (calibrate-methods), 33
calibrate,XCMSnExp-method (CalibrantMassParam-class), 31
calibrate,xcmsSet-method (calibrate-methods), 33
calibrate-methods, 33

centerSample (adjustRtime), 7
centerSample,ObiwarpParam-method (adjustRtime), 7
centerSample<- (adjustRtime), 7
centerSample<-,ObiwarpParam-method (adjustRtime), 7
centWave, *56*, *59*, *119*, *120*, *132*, *161*, *166*, *214*, *215*
centWave (findChromPeaks-centWave), 122
CentWaveParam, *119*, *120*, *129*, *133*, *146*, *171*, *243*, *311*
CentWaveParam (findChromPeaks-centWave), 122
CentWaveParam(), *117*
CentWaveParam-class (findChromPeaks-centWave), 122
CentWavePredIsoParam, *311*
CentWavePredIsoParam (findChromPeaks-centWaveWithPredIsoROIs), 128
CentWavePredIsoParam(), *117*
CentWavePredIsoParam-class (findChromPeaks-centWaveWithPredIsoROIs), 128
centWaveWithPredIsoROIs (findChromPeaks-centWaveWithPredIsoROIs), 128
character, *302*
CharacterList(), *257*
checkBack (findChromPeaks-massifquant), 133
checkBack,MassifquantParam-method (findChromPeaks-massifquant), 133
checkBack<- (findChromPeaks-massifquant), 133
checkBack<-,MassifquantParam-method (findChromPeaks-massifquant), 133
Chromatogram, *36*, *119–121*, *195*, *295*, *313*, *314*
chromatogram, *314*
chromatogram (chromatogram,XCMSnExp-method), 34
Chromatogram(), *45*, *97*, *264*, *288*
chromatogram(), *83*, *295*, *297*
chromatogram,MsExperiment-method (filterFeatureDefinitions), 99
chromatogram,XcmsExperiment-method (filterFeatureDefinitions), 99
chromatogram,XCMSnExp-method, 34
ChromPeakAreaParam (fillChromPeaks), 89
ChromPeakAreaParam-class (fillChromPeaks), 89
chromPeakChromatograms, 37
chromPeakChromatograms(), *84*
chromPeakChromatograms,XcmsExperiment-method (chromPeakChromatograms), 37
chromPeakData (XCMSnExp-class), 305
chromPeakData(), *89*, *145*, *147*
chromPeakData,MsFeatureData-method (XCMSnExp-class), 305
chromPeakData,XChromatogram-method (XChromatograms), 288
chromPeakData,XChromatograms-method (XChromatograms), 288
chromPeakData,XcmsExperiment-method (filterFeatureDefinitions), 99
chromPeakData,XCMSnExp-method (XCMSnExp-class), 305
chromPeakData<- (XCMSnExp-class), 305
chromPeakData<-,MsFeatureData-method (XCMSnExp-class), 305
chromPeakData<-,XChromatogram-method (XChromatograms), 288
chromPeakData<-,XcmsExperiment-method (filterFeatureDefinitions), 99
chromPeakData<-,XCMSnExp-method (XCMSnExp-class), 305
chromPeaks, *196*, *230*, *251*
chromPeaks (XCMSnExp-class), 305
chromPeaks(), *40*, *89*, *92*, *145*
chromPeaks,MsFeatureData-method (XCMSnExp-class), 305
chromPeaks,XChromatogram-method (XChromatograms), 288
chromPeaks,XChromatograms-method (XChromatograms), 288
chromPeaks,XcmsExperiment-method (filterFeatureDefinitions), 99
chromPeaks,XCMSnExp-method (XCMSnExp-class), 305
chromPeaks<- (XCMSnExp-class), 305
chromPeaks<-,MsFeatureData-method

(XCMSnExp-class), 305
chromPeaks<-,XChromatogram-method (XChromatograms), 288
chromPeaks<-,XcmsExperiment-method (filterFeatureDefinitions), 99
chromPeaks<-,XCMSnExp-method (XCMSnExp-class), 305
chromPeakSpectra, 38, *314*
chromPeakSpectra(), *86, 87*, *109*
chromPeakSpectra,XcmsExperiment-method (chromPeakSpectra), 38
chromPeakSpectra,XCMSnExp-method (chromPeakSpectra), 38
class:Param (GenericParam-class), 171
clean, *21*
clean(), *263*
clean,XCMSnExp-method (bin,XCMSnExp-method), 21
CleanPeaksParam (refineChromPeaks), 259
CleanPeaksParam-class (refineChromPeaks), 259
coerce,MChromatograms,XChromatograms-method (XChromatograms), 288
collect, *303, 304*
collect (collect-methods), 42
collect,xcmsFragments-method (collect-methods), 42
collect,xcmsRaw-method (collect-methods), 42
collect-methods, 42
colMax, 43
colSums, *43*
compareChromatograms(), *44*, *188, 189*
consecMissedLimit (findChromPeaks-massifquant), 133
consecMissedLimit,MassifquantParam-method (findChromPeaks-massifquant), 133
consecMissedLimit<- (findChromPeaks-massifquant), 133
consecMissedLimit<-,MassifquantParam-method (findChromPeaks-massifquant), 133
cor(), *45*, *189*
correlate (correlate,Chromatogram,Chromatogram-method), 44
correlate,Chromatogram,Chromatogram-method, 44
correlate,MChromatograms,MChromatograms-method (correlate,Chromatogram,Chromatogram-method), 44
correlate,MChromatograms,missing-method (correlate,Chromatogram,Chromatogram-method), 44
criticalValue (findChromPeaks-massifquant), 133
criticalValue,MassifquantParam-method (findChromPeaks-massifquant), 133
criticalValue<- (findChromPeaks-massifquant), 133
criticalValue<-,MassifquantParam-method (findChromPeaks-massifquant), 133

DataFrame(), *295*
deepCopy (xcmsRaw), 317
deepCopy,xcmsRaw-method (xcmsRaw), 317
density, *177*
descendMin (descendZero), 46
descendValue, *46*
descendValue (descendZero), 46
descendZero, 46
diffreport, *7*, *217*, *324*
diffreport (diffreport-methods), 47
diffreport,xcmsSet-method (diffreport-methods), 47
diffreport-methods, 47
dirname, 49
dirname,OnDiskMSnExp-method (dirname), 49
dirname<-,OnDiskMSnExp-method (dirname), 49
distance (findChromPeaks-matchedFilter), 140
distance,MatchedFilterParam-method (findChromPeaks-matchedFilter), 140
distance<- (findChromPeaks-matchedFilter), 140

distance<-,MatchedFilterParam-method
(findChromPeaks-matchedFilter), 140
distFun (adjustRtime), 7
distFun,ObiwarpParam-method
(adjustRtime), 7
distFun<- (adjustRtime), 7
distFun<-,ObiwarpParam-method
(adjustRtime), 7
do_adjustRtime_peakGroups, 50
do_adjustRtime_peakGroups(), *8*
do_findChromPeaks_addPredIsoROIs
(do_findChromPeaks_centWaveWithPredIsoROIs), 56
do_findChromPeaks_centWave, 52, *60, 61*, *63, 64*, *67*, *69*, *128*, *137*
do_findChromPeaks_centWaveWithPredIsoROIs, *56*, 56, *64*, *67*, *69*, *133*, *163*
do_findChromPeaks_massifquant, *56*, *60*, 61, *67*, *69*, *139*
do_findChromPeaks_matchedFilter, *56*, *60*, *64*, 64, *69*, *145*, *166*, *168*, *283*
do_findPeaks_MSW, *56*, *60*, *64*, *67*, 67, *156*, *171*
do_groupChromPeaks_density, 69, *73*, *75*, *177*
do_groupChromPeaks_density(), *181*
do_groupChromPeaks_nearest, *71*, 72, *75*
do_groupChromPeaks_nearest(), *181*
do_groupPeaks_mzClust, *71*, *73*, 73
do_groupPeaks_mzClust(), *181*
doubleMatrix, 49
DratioFilter, *27, 28*, 75, *76*, *115*, *219*, *270, 271*
dropAdjustedRtime (XCMSnExp-class), 305
dropAdjustedRtime(), *19*
dropAdjustedRtime,MsFeatureData-method
(XCMSnExp-class), 305
dropAdjustedRtime,XcmsExperiment-method
(filterFeatureDefinitions), 99
dropAdjustedRtime,XCMSnExp-method
(XCMSnExp-class), 305
dropChromPeaks (XCMSnExp-class), 305
dropChromPeaks,MsFeatureData-method
(XCMSnExp-class), 305
dropChromPeaks,XcmsExperiment-method
(filterFeatureDefinitions), 99
dropChromPeaks,XCMSnExp-method
(XCMSnExp-class), 305
dropFeatureDefinitions
(XCMSnExp-class), 305
dropFeatureDefinitions,MsFeatureData-method
(XCMSnExp-class), 305
dropFeatureDefinitions,XChromatograms-method
(XChromatograms), 288
dropFeatureDefinitions,XcmsExperiment-method
(filterFeatureDefinitions), 99
dropFeatureDefinitions,XCMSnExp-method
(XCMSnExp-class), 305
dropFilledChromPeaks (XCMSnExp-class), 305
dropFilledChromPeaks(), *296*
dropFilledChromPeaks,XChromatogram-method
(XChromatograms), 288
dropFilledChromPeaks,XChromatograms-method
(XChromatograms), 288
dropFilledChromPeaks,XcmsExperiment-method
(filterFeatureDefinitions), 99
dropFilledChromPeaks,XCMSnExp-method
(XCMSnExp-class), 305

EicSimilarityParam
(groupFeatures-eic-similarity), 187
EicSimilarityParam(), *81*
EicSimilarityParam-class
(groupFeatures-eic-similarity), 187
estimatePrecursorIntensity, 76
etg, 77
expandMz (fillChromPeaks), 89
expandMz,FillChromPeaksParam-method
(fillChromPeaks), 89
expandMz<- (fillChromPeaks), 89
expandMz<-,FillChromPeaksParam-method
(fillChromPeaks), 89
expandRt (fillChromPeaks), 89
expandRt,FillChromPeaksParam-method
(fillChromPeaks), 89
expandRt<- (fillChromPeaks), 89
expandRt<-,FillChromPeaksParam-method
(fillChromPeaks), 89
exportMetaboAnalyst, 78
extractMsData
(extractMsData,OnDiskMSnExp-method), 79
extractMsData(), *235*

extractMsData,OnDiskMSnExp-method, 79
extractMsData,XCMSnExp-method
(extractMsData,OnDiskMSnExp-method), 79
extraPeaks (adjustRtime), 7
extraPeaks,PeakGroupsParam-method
(adjustRtime), 7
extraPeaks<- (adjustRtime), 7
extraPeaks<-,PeakGroupsParam-method
(adjustRtime), 7

faahko_sub (loadXcmsData), 204
faahko_sub2 (loadXcmsData), 204
factorDiag (adjustRtime), 7
factorDiag,ObiwarpParam-method
(adjustRtime), 7
factorDiag<- (adjustRtime), 7
factorDiag<-,ObiwarpParam-method
(adjustRtime), 7
factorGap (adjustRtime), 7
factorGap,ObiwarpParam-method
(adjustRtime), 7
factorGap<- (adjustRtime), 7
factorGap<-,ObiwarpParam-method
(adjustRtime), 7
family (adjustRtime), 7
family,PeakGroupsParam-method
(adjustRtime), 7
family<- (adjustRtime), 7
family<-,PeakGroupsParam-method
(adjustRtime), 7
feature-grouping, 81
featureArea, *93*
featureArea (filterFeatureDefinitions), 99
featureChromatograms, 82, *253*, *314*
featureChromatograms(), *38*, *110*, *189*
featureChromatograms,XcmsExperiment-method
(featureChromatograms), 82
featureChromatograms,XCMSnExp-method
(featureChromatograms), 82
featureDefinitions, *251*, *253*, *314*
featureDefinitions (XCMSnExp-class), 305
featureDefinitions(), *89*, *191*, *211*
featureDefinitions,MsFeatureData-method
(XCMSnExp-class), 305
featureDefinitions,XChromatograms-method
(XChromatograms), 288
featureDefinitions,XcmsExperiment-method
(filterFeatureDefinitions), 99
featureDefinitions,XCMSnExp-method
(XCMSnExp-class), 305
featureDefinitions<- (XCMSnExp-class), 305
featureDefinitions<-,MsFeatureData-method
(XCMSnExp-class), 305
featureDefinitions<-,XcmsExperiment-method
(filterFeatureDefinitions), 99
featureDefinitions<-,XCMSnExp-method
(XCMSnExp-class), 305
featureGroups(), *234*
featureGroups,XcmsResult-method
(feature-grouping), 81
featureGroups<-,XcmsResult-method
(feature-grouping), 81
featureSpectra, 85, *314*
featureSpectra(), *110*
featureSpectra,XcmsExperiment-method
(featureSpectra), 85
featureSpectra,XCMSnExp-method
(featureSpectra), 85
featureSummary, 87, *305*, *314*
featureSummary(), *110*
featureValues, *251, 252*, *314*
featureValues
(quantify,XCMSnExp-method), 251
featureValues(), *27*, *76*, *79*, *93*, *115*, *186*, *219*, *270*
featureValues,XChromatograms-method
(XChromatograms), 288
featureValues,XcmsExperiment-method
(filterFeatureDefinitions), 99
featureValues,XCMSnExp-method
(quantify,XCMSnExp-method), 251
fileIndex (ProcessHistory-class), 242
fileIndex,ProcessHistory-method
(ProcessHistory-class), 242
fileNames,MsExperiment-method
(filterFeatureDefinitions), 99
filepaths (xcmsSet-class), 323
filepaths,xcmsSet-method
(xcmsSet-class), 323
filepaths<- (xcmsSet-class), 323
filepaths<-,xcmsSet-method
(xcmsSet-class), 323
fillChromPeaks, 89, *252*, *307*, *313, 314*

fillChromPeaks(), *100*, *109*
fillChromPeaks,XcmsExperiment,ChromPeakAreaParam-method *(fillChromPeaks)*, 89
fillChromPeaks,XCMSnExp,ChromPeakAreaParam-method *(fillChromPeaks)*, 89
fillChromPeaks,XCMSnExp,FillChromPeaksParam-method *(fillChromPeaks)*, 89
fillChromPeaks,XCMSnExp,missing-method *(fillChromPeaks)*, 89
FillChromPeaksParam *(fillChromPeaks)*, 89
FillChromPeaksParam-class *(fillChromPeaks)*, 89
fillPeaks, *7*, *47*, *96*, *324*
fillPeaks *(fillPeaks-methods)*, 94
fillPeaks,xcmsSet-method *(fillPeaks-methods)*, 94
fillPeaks-methods, 94
fillPeaks.chrom, *96*
fillPeaks.chrom *(fillPeaks.chrom-methods)*, 95
fillPeaks.chrom,xcmsSet-method *(fillPeaks.chrom-methods)*, 95
fillPeaks.chrom-methods, 95
fillPeaks.MSW *(fillPeaks.MSW-methods)*, 96
fillPeaks.MSW,xcmsSet-method *(fillPeaks.MSW-methods)*, 96
fillPeaks.MSW-methods, 96
filterAcquisitionNum, *21*
filterAcquisitionNum,XCMSnExp-method *(bin,XCMSnExp-method)*, 21
filterChromPeaks *(filterFeatureDefinitions)*, 99
filterChromPeaks,XChromatogram-method *(XChromatograms)*, 288
filterChromPeaks,XChromatograms-method *(XChromatograms)*, 288
filterChromPeaks,XcmsExperiment-method *(filterFeatureDefinitions)*, 99
filterChromPeaks,XCMSnExp-method *([,XCMSnExp,ANY,ANY,ANY-method)*, 327
filterColumnsIntensityAbove *(filterColumnsIntensityAbove,MChromatograms-method)*, 97
filterColumnsIntensityAbove(), *295*
filterColumnsIntensityAbove,MChromatograms-method, 97
filterColumnsIntensityAbove,XChromatograms-method *(filterColumnsIntensityAbove,MChromatograms-method)*, 97
filterColumnsKeepTop *(filterColumnsIntensityAbove,MChromatograms-method)*, 97
filterColumnsKeepTop(), *84*
filterColumnsKeepTop,MChromatograms-method *(filterColumnsIntensityAbove,MChromatograms-method)*, 97
filterColumnsKeepTop,XChromatograms-method *(filterColumnsIntensityAbove,MChromatograms-method)*, 97
filterFeatureDefinitions, 99
filterFeatureDefinitions,XcmsExperiment-method *(filterFeatureDefinitions)*, 99
filterFeatureDefinitions,XCMSnExp-method *([,XCMSnExp,ANY,ANY,ANY-method)*, 327
filterFeatures, 115
filterFeatures,SummarizedExperiment,BlankFlag-method *(BlankFlag)*, 26
filterFeatures,SummarizedExperiment,DratioFilter-method *(DratioFilter)*, 75
filterFeatures,SummarizedExperiment,PercentMissingFilter-m *(PercentMissingFilter)*, 218
filterFeatures,SummarizedExperiment,RsdFilter-method *(RsdFilter)*, 269
filterFeatures,XcmsResult,BlankFlag-method *(BlankFlag)*, 26
filterFeatures,XcmsResult,DratioFilter-method *(DratioFilter)*, 75
filterFeatures,XcmsResult,PercentMissingFilter-method *(PercentMissingFilter)*, 218
filterFeatures,XcmsResult,RsdFilter-method *(RsdFilter)*, 269
filterFile,MsExperiment-method *(filterFeatureDefinitions)*, 99
filterFile,XcmsExperiment-method *(filterFeatureDefinitions)*, 99
filterFile,XCMSnExp-method *([,XCMSnExp,ANY,ANY,ANY-method)*, 327
filterIntensity(), *264*
FilterIntensityParam *(refineChromPeaks)*, 259
FilterIntensityParam-class *(refineChromPeaks)*, 259

filterIsolationWindow,MsExperiment-method (filterFeatureDefinitions), 99
filterIsolationWindow,XcmsExperiment-method (filterFeatureDefinitions), 99
filterMsLevel,MsExperiment-method (filterFeatureDefinitions), 99
filterMsLevel,XcmsExperiment-method (filterFeatureDefinitions), 99
filterMsLevel,XCMSnExp-method ([,XCMSnExp,ANY,ANY,ANY-method), 327
filterMz,MsExperiment-method (filterFeatureDefinitions), 99
filterMz,XChromatogram-method (XChromatograms), 288
filterMz,XChromatograms-method (XChromatograms), 288
filterMz,XCMSnExp-method ([,XCMSnExp,ANY,ANY,ANY-method), 327
filterMzRange,MsExperiment-method (filterFeatureDefinitions), 99
filterMzRange,XcmsExperiment-method (filterFeatureDefinitions), 99
filterRt,MsExperiment-method (filterFeatureDefinitions), 99
filterRt,XChromatogram-method (XChromatograms), 288
filterRt,XChromatograms-method (XChromatograms), 288
filterRt,XcmsExperiment-method (filterFeatureDefinitions), 99
filterRt,XCMSnExp-method ([,XCMSnExp,ANY,ANY,ANY-method), 327
filtfft, 117
findChromPeaks, 117, *128*, *133*, *139*, *145*, *156*, *242*, *306*, *313*, *314*
findChromPeaks(), *100*, *108*, *109*, *145*, *146*, *259*
findChromPeaks,Chromatogram,CentWaveParam-method, 119
findChromPeaks,Chromatogram,MatchedFilterParam-method, 121
findChromPeaks,MChromatograms,CentWaveParam-method (findChromPeaks,Chromatogram,CentWaveParam-method), 119
findChromPeaks,MChromatograms,MatchedFilterParam-method (findChromPeaks,Chromatogram,CentWaveParam-method), 119
findChromPeaks,MsExperiment,Param-method (findChromPeaks), 117
findChromPeaks,OnDiskMSnExp,CentWaveParam-method (findChromPeaks-centWave), 122
findChromPeaks,OnDiskMSnExp,CentWavePredIsoParam-method (findChromPeaks-centWaveWithPredIsoROIs), 128
findChromPeaks,OnDiskMSnExp,MassifquantParam-method (findChromPeaks-massifquant), 133
findChromPeaks,OnDiskMSnExp,MatchedFilterParam-method (findChromPeaks-matchedFilter), 140
findChromPeaks,OnDiskMSnExp,MSWParam-method (findPeaks-MSW), 152
findChromPeaks,XcmsExperiment,Param-method (findChromPeaks), 117
findChromPeaks,XCMSnExp,Param-method (XCMSnExp-class), 305
findChromPeaks-centWave, 122, *298*
findChromPeaks-centWaveWithPredIsoROIs, 128
findChromPeaks-Chromatogram-CentWaveParam, *297*
findChromPeaks-Chromatogram-CentWaveParam (findChromPeaks,Chromatogram,CentWaveParam-method), 119
findChromPeaks-massifquant, 133
findChromPeaks-matchedFilter, 140
findChromPeaksIsolationWindow, 145
findChromPeaksIsolationWindow(), *258*
findChromPeaksIsolationWindow,MsExperiment-method (findChromPeaksIsolationWindow), 145
findChromPeaksIsolationWindow,OnDiskMSnExp-method (findChromPeaksIsolationWindow), 145
findEqualGreater, 147
findEqualGreaterM (findEqualGreater), 147
findEqualLess (findEqualGreater), 147
findMZ, 148, *150*
findMZ,xcmsFragments-method (findMZ), 148
findmzROI (xcmsRaw-class), 319
findmzROI,xcmsRaw-method

(xcmsRaw-class), 319
findneutral, *149*, 149
findneutral,xcmsFragments-method (findneutral), 149
findPeaks, *127*, *133*, *139*, *144*, *155*, *173*, *212*, *236*, *248*, *271*, *316*, *320*, *323*
findPeaks (findPeaks-methods), 151
findPeaks,xcmsRaw-method (findPeaks-methods), 151
findPeaks-methods, 151
findPeaks-MSW, 152
findPeaks.addPredictedIsotopeFeatures, *151*, *163*
findPeaks.addPredictedIsotopeFeatures (findPeaks.addPredictedIsotopeFeatures-methods), 156
findPeaks.addPredictedIsotopeFeatures,xcmsRaw-method (findPeaks.addPredictedIsotopeFeatures-methods), 156
findPeaks.addPredictedIsotopeFeatures-methods, 156
findPeaks.centWave, *47*, *128*, *133*, *151*, *158*, *163*
findPeaks.centWave (findPeaks.centWave-methods), 159
findPeaks.centWave,xcmsRaw-method (findPeaks.centWave-methods), 159
findPeaks.centWave-methods, 159
findPeaks.centWaveWithPredictedIsotopeROIs, *151*
findPeaks.centWaveWithPredictedIsotopeROIs (findPeaks.centWaveWithPredictedIsotopeROIs-methods), 161
findPeaks.centWaveWithPredictedIsotopeROIs,xcmsRaw-method (findPeaks.centWaveWithPredictedIsotopeROIs-methods), 161
findPeaks.centWaveWithPredictedIsotopeROIs-methods, 161
findPeaks.massifquant, *139*
findPeaks.massifquant (findPeaks.massifquant-methods), 164
findPeaks.massifquant,xcmsRaw-method (findPeaks.massifquant-methods), 164
findPeaks.massifquant-methods, 164
findPeaks.matchedFilter, *145*, *151*, *323*
findPeaks.matchedFilter (findPeaks.matchedFilter,xcmsRaw-method), 166
findPeaks.matchedFilter,xcmsRaw-method, 166
findPeaks.MS1 (findPeaks.MS1-methods), 168
findPeaks.MS1,xcmsRaw-method (findPeaks.MS1-methods), 168
findPeaks.MS1-methods, 168
findPeaks.MSW, *156*
findPeaks.MSW (findPeaks.MSW,xcmsRaw-method), 170
findPeaks.MSW,xcmsRaw-method, 170
findRange (findEqualGreater), 147
firstBaselineCheck (findChromPeaks-centWave), 122
firstBaselineCheck,CentWaveParam-method (findChromPeaks-centWave), 122
firstBaselineCheck<- (findChromPeaks-centWave), 122
firstBaselineCheck<-,CentWaveParam-method (findChromPeaks-centWave), 122
fitgauss (findChromPeaks-centWave), 122
fitgauss,CentWaveParam-method (findChromPeaks-centWave), 122
fitgauss,MassifquantParam-method (findChromPeaks-massifquant), 133
fitgauss<- (findChromPeaks-centWave), 122
fitgauss<-,CentWaveParam-method (findChromPeaks-centWave), 122
fitgauss<-,MassifquantParam-method (findChromPeaks-massifquant), 133
fixedMz (fillChromPeaks), 89
fixedRt (fillChromPeaks), 89
format(), *79*
fromFile,MsExperiment-method (filterFeatureDefinitions), 99
fwhm (findChromPeaks-matchedFilter), 140
fwhm,MatchedFilterParam-method (findChromPeaks-matchedFilter), 140
fwhm<- (findChromPeaks-matchedFilter),

140
fwhm<-,MatchedFilterParam-method (findChromPeaks-matchedFilter), 140

gapExtend (adjustRtime), 7
gapExtend,ObiwarpParam-method (adjustRtime), 7
gapExtend<- (adjustRtime), 7
gapExtend<-,ObiwarpParam-method (adjustRtime), 7
gapInit (adjustRtime), 7
gapInit,ObiwarpParam-method (adjustRtime), 7
gapInit<- (adjustRtime), 7
gapInit<-,ObiwarpParam-method (adjustRtime), 7
GenericParam (GenericParam-class), 171
GenericParam-class, 171
getEIC, *253*, *268*, *301*, *302*, *320*, *324*
getEIC (getEIC-methods), 172
getEIC,xcmsRaw-method (getEIC-methods), 172
getEIC,xcmsSet-method (getEIC-methods), 172
getEIC-methods, 172
getMsnScan (getScan-methods), 174
getMsnScan,xcmsRaw-method (getScan-methods), 174
getPeaks, *94*, *96*, *283*, *320*
getPeaks (getPeaks-methods), 173
getPeaks,xcmsRaw-method (getPeaks-methods), 173
getPeaks-methods, 173
getScan, *175*, *320*
getScan (getScan-methods), 174
getScan,xcmsRaw-method (getScan-methods), 174
getScan-methods, 174
getSpec, *174*, *276*, *277*, *320*
getSpec (getSpec-methods), 174
getSpec,xcmsRaw-method (getSpec-methods), 174
getSpec-methods, 174
getXcmsRaw, *324*
getXcmsRaw (getXcmsRaw-methods), 175
getXcmsRaw,xcmsSet-method (getXcmsRaw-methods), 175
getXcmsRaw-methods, 175

group, *7*, *323*, *325*
group (group-methods), 176
group,xcmsSet-method (group-methods), 176
group-methods, 176
group.density, *176*, 177, *179*
group.density,xcmsSet-method (group.density), 177
group.mzClust, *176*, 178, *179*
group.mzClust,xcmsSet-method (group.mzClust), 178
group.nearest, *176*, 179
group.nearest,xcmsSet-method (group.nearest), 179
groupChromPeaks, 180, *297*, *314*
groupChromPeaks(), *8*, *81*, *93*, *100*, *110*, *230*
groupChromPeaks,XChromatograms,PeakDensityParam-method (XChromatograms), 288
groupChromPeaks,XcmsExperiment,Param-method (groupChromPeaks), 180
groupChromPeaks,XCMSnExp,MzClustParam-method (groupChromPeaks), 180
groupChromPeaks,XCMSnExp,NearestPeaksParam-method (groupChromPeaks), 180
groupChromPeaks,XCMSnExp,PeakDensityParam-method (groupChromPeaks), 180
groupFeatures(), *234*
groupFeatures,XcmsResult,AbundanceSimilarityParam-method (groupFeatures-abundance-correlation), 186
groupFeatures,XcmsResult,EicSimilarityParam-method (groupFeatures-eic-similarity), 187
groupFeatures,XcmsResult,SimilarRtimeParam-method (groupFeatures-similar-rtime), 191
groupFeatures-abundance-correlation, 186
groupFeatures-eic-similarity, 187
groupFeatures-similar-rtime, 191
groupidx (xcmsSet-class), 323
groupidx,xcmsSet-method (xcmsSet-class), 323
groupidx<- (xcmsSet-class), 323
groupidx<-,xcmsSet-method (xcmsSet-class), 323
groupnames, *79*, *301*, *325*
groupnames (groupnames-methods), 193

groupnames,xcmsEIC-method
(groupnames-methods), 193
groupnames,XCMSnExp-method, 192
groupnames,xcmsSet-method
(groupnames-methods), 193
groupnames-methods, 193
groupOverlaps, 193
groups (xcmsSet-class), 323
groups,xcmsSet-method (xcmsSet-class),
323
groups<- (xcmsSet-class), 323
groups<-,xcmsSet-method
(xcmsSet-class), 323
groupSimilarityMatrix(), *188*, *189*
groupval, *217*, *253*, *325*
groupval (groupval-methods), 194
groupval,xcmsSet-method
(groupval-methods), 194
groupval-methods, 194

hasAdjustedRtime (XCMSnExp-class), 305
hasAdjustedRtime,MsExperiment-method
(filterFeatureDefinitions), 99
hasAdjustedRtime,MsFeatureData-method
(XCMSnExp-class), 305
hasAdjustedRtime,OnDiskMSnExp-method
(XCMSnExp-class), 305
hasAdjustedRtime,XCMSnExp-method
(XCMSnExp-class), 305
hasChromPeaks (XCMSnExp-class), 305
hasChromPeaks,MsFeatureData-method
(XCMSnExp-class), 305
hasChromPeaks,XChromatogram-method
(XChromatograms), 288
hasChromPeaks,XChromatograms-method
(XChromatograms), 288
hasChromPeaks,XcmsExperiment-method
(filterFeatureDefinitions), 99
hasChromPeaks,XCMSnExp-method
(XCMSnExp-class), 305
hasFeatures, *253*
hasFeatures (XCMSnExp-class), 305
hasFeatures,MsFeatureData-method
(XCMSnExp-class), 305
hasFeatures,XChromatograms-method
(XChromatograms), 288
hasFeatures,XcmsExperiment-method
(filterFeatureDefinitions), 99
hasFeatures,XCMSnExp-method
(XCMSnExp-class), 305
hasFilledChromPeaks (XCMSnExp-class),
305
hasFilledChromPeaks,XChromatograms-method
(XChromatograms), 288
hasFilledChromPeaks,XcmsExperiment-method
(filterFeatureDefinitions), 99
hasFilledChromPeaks,XCMSnExp-method
(XCMSnExp-class), 305
highlightChromPeaks, 195, *313*

identifyMajorPeaks, *152*, *155*, *170*
image, *320*
image,xcmsRaw-method (image-methods),
197
image-methods, 197
impute,MatchedFilterParam-method
(findChromPeaks-matchedFilter),
140
impute<-
(findChromPeaks-matchedFilter),
140
impute<-,MatchedFilterParam-method
(findChromPeaks-matchedFilter),
140
imputeLinInterpol, *25*, *65–67*, *143*, *144*,
197, *245*, *301*
imputeLinInterpol(), *246*, *247*, *310*
imputeRowMin, 199, *201*
imputeRowMinRand, *200*, 200
index (findChromPeaks-matchedFilter),
140
index,MatchedFilterParam-method
(findChromPeaks-matchedFilter),
140
index<- (findChromPeaks-matchedFilter),
140
index<-,MatchedFilterParam-method
(findChromPeaks-matchedFilter),
140
initPenalty (adjustRtime), 7
initPenalty,ObiwarpParam-method
(adjustRtime), 7
initPenalty<- (adjustRtime), 7
initPenalty<-,ObiwarpParam-method
(adjustRtime), 7
integerMatrix (doubleMatrix), 49

integrate,CentWaveParam-method
(findChromPeaks-centWave), 122
integrate,MassifquantParam-method
(findChromPeaks-massifquant),
133
integrate<- (findChromPeaks-centWave),
122
integrate<-,CentWaveParam-method
(findChromPeaks-centWave), 122
integrate<-,MassifquantParam-method
(findChromPeaks-massifquant),
133
intensity,XCMSnExp-method
(XCMSnExp-class), 305
isCalibrated
(CalibrantMassParam-class), 31
isolationWindowTargetMz
(isolationWindowTargetMz,OnDiskMSnExp-method),
202
isolationWindowTargetMz(), *146*
isolationWindowTargetMz,OnDiskMSnExp-method,
202

kNN (groupChromPeaks), 180
kNN,NearestPeaksParam-method
(groupChromPeaks), 180
kNN<- (groupChromPeaks), 180
kNN<-,NearestPeaksParam-method
(groupChromPeaks), 180

LamaParama
(adjustRtime,XcmsExperiment,LamaParama-method),
15
LamaParama(), *8*
LamaParama-class
(adjustRtime,XcmsExperiment,LamaParama-method),
15
lattice::level.colors, *235*
levelplot, *320*
levelplot (xcmsRaw-class), 319
levelplot,xcmsRaw-method
(levelplot-methods), 203
levelplot,xcmsSet-method
(levelplot-methods), 203
levelplot-methods, 203
loadRaw (loadRaw-methods), 203
loadRaw,xcmsFileSource-method
(loadRaw-methods), 203
loadRaw,xcmsSource-method
(loadRaw-methods), 203
loadRaw-methods, 203
loadXcmsData, 204
localAlignment (adjustRtime), 7
localAlignment,ObiwarpParam-method
(adjustRtime), 7
localAlignment<- (adjustRtime), 7
localAlignment<-,ObiwarpParam-method
(adjustRtime), 7
loess, *267*
loess(), *12*, *51*
logicalMatrix (doubleMatrix), 49

makeacqNum (stitch-methods), 279
makeacqNum, xcmsRaw-method
(stitch-methods), 279
manualChromPeaks, 205
manualChromPeaks(), *109*, *119*
manualChromPeaks,MsExperiment-method
(manualChromPeaks), 205
manualChromPeaks,OnDiskMSnExp-method
(manualChromPeaks), 205
manualChromPeaks,XcmsExperiment-method
(manualChromPeaks), 205
manualChromPeaks,XCMSnExp-method
(manualChromPeaks), 205
manualFeatures (manualChromPeaks), 205
manualFeatures,XcmsExperiment-method
(manualChromPeaks), 205
manualFeatures,XCMSnExp-method
(manualChromPeaks), 205
massifquant, *64*
massifquant
(findChromPeaks-massifquant),
133
MassifquantParam, *311*
MassifquantParam
(findChromPeaks-massifquant),
133
MassifquantParam(), *117*
MassifquantParam-class
(findChromPeaks-massifquant),
133
matchedFilter, *67*, *121*, *122*, *168*, *215*, *216*
matchedFilter
(findChromPeaks-matchedFilter),
140
matchedFilter(), *92*

MatchedFilterParam, *121*, *311*
MatchedFilterParam (findChromPeaks-matchedFilter), 140
MatchedFilterParam(), *117*
MatchedFilterParam-class (findChromPeaks-matchedFilter), 140
matchedRtimes (adjustRtime,XcmsExperiment,LamaParameters-method), 15
matchLamasChromPeaks (adjustRtime,XcmsExperiment,LamaParameters-method), 15
matplot, *196*
matrix, *316*
max,MatchedFilterParam-method (findChromPeaks-matchedFilter), 140
max<- (findChromPeaks-matchedFilter), 140
max<-,MatchedFilterParam-method (findChromPeaks-matchedFilter), 140
maxCharge (findChromPeaks-centWaveWithPredIsoROIs), 128
maxCharge,CentWavePredIsoParam-method (findChromPeaks-centWaveWithPredIsoROIs), 128
maxCharge<- (findChromPeaks-centWaveWithPredIsoROIs), 128
maxCharge<-,CentWavePredIsoParam-method (findChromPeaks-centWaveWithPredIsoROIs), 128
maxFeatures (groupChromPeaks), 180
maxFeatures,PeakDensityParam-method (groupChromPeaks), 180
maxFeatures<- (groupChromPeaks), 180
maxFeatures<-,PeakDensityParam-method (groupChromPeaks), 180
maxIso (findChromPeaks-centWaveWithPredIsoROIs), 128
maxIso,CentWavePredIsoParam-method (findChromPeaks-centWaveWithPredIsoROIs), 128
maxIso<- (findChromPeaks-centWaveWithPredIsoROIs), 128
maxIso<-,CentWavePredIsoParam-method (findChromPeaks-centWaveWithPredIsoROIs), 128
MChromatograms, *35*, *119–121*, *195*
MChromatograms(), *44*, *45*, *97*, *98*, *108*, *118*, *225*, *226*, *264*, *288*, *295*, *298*
medianFilter, 208, *248*
MergeNeighboringPeaksParam (refineChromPeaks), 259
MergeNeighboringPeaksParam(), *205*, *297*
MergeNeighboringPeaksParam-class (refineChromPeaks), 259
minFraction (groupChromPeaks), 180
minFraction,MzClustParam-method (groupChromPeaks), 180
minFraction,PeakDensityParam-method (groupChromPeaks), 180
minFraction,PeakGroupsParam-method (adjustRtime), 7
minFraction<- (groupChromPeaks), 180
minFraction<-,MzClustParam-method (groupChromPeaks), 180
minFraction<-,PeakDensityParam-method (groupChromPeaks), 180
minFraction<-,PeakGroupsParam-method (adjustRtime), 7
minNoiseLevel (findPeaks-MSW), 152
minNoiseLevel,MSWParam-method (findPeaks-MSW), 152
minNoiseLevel<- (findPeaks-MSW), 152
minNoiseLevel<-,MSWParam-method (findPeaks-MSW), 152
minSamples (groupChromPeaks), 180
minSamples,MzClustParam-method (groupChromPeaks), 180
minSamples,PeakDensityParam-method (groupChromPeaks), 180
minSamples<- (groupChromPeaks), 180
minSamples<-,MzClustParam-method (groupChromPeaks), 180
minSamples<-,PeakDensityParam-method (groupChromPeaks), 180
MsExperiment(), *12*, *118*
MsFeatures::groupFeatures(), *81*
MsFeatures::SimilarRtimeParam(), *191*

mslevel (xcmsSet-class), 323
mslevel,xcmsRaw-method (xcmsRaw-class), 319
mslevel,xcmsSet-method (xcmsSet-class), 323
msLevel,XProcessHistory-method (ProcessHistory-class), 242
msn2xcmsRaw, 209
MSnbase::Chromatogram(), *44*, *45*
MSnExp, *307*, *314*
MSpectra, *40*
MSW, *69*, *171*
MSW (findPeaks-MSW), 152
MSWParam, *311*
MSWParam (findPeaks-MSW), 152
MSWParam(), *117*
MSWParam-class (findPeaks-MSW), 152
MulticoreParam, *322*
mz,CalibrantMassParam (CalibrantMassParam-class), 31
mz,XCMSnExp-method (XCMSnExp-class), 305
mzCenterFun (findChromPeaks-centWave), 122
mzCenterFun,CentWaveParam-method (findChromPeaks-centWave), 122
mzCenterFun,MassifquantParam-method (findChromPeaks-massifquant), 133
mzCenterFun<- (findChromPeaks-centWave), 122
mzCenterFun<-,CentWaveParam-method (findChromPeaks-centWave), 122
mzCenterFun<-,MassifquantParam-method (findChromPeaks-massifquant), 133
MzClustParam (groupChromPeaks), 180
MzClustParam-class (groupChromPeaks), 180
mzdiff (findChromPeaks-centWave), 122
mzdiff,CentWaveParam-method (findChromPeaks-centWave), 122
mzdiff,MassifquantParam-method (findChromPeaks-massifquant), 133
mzdiff,MatchedFilterParam-method (findChromPeaks-matchedFilter), 140
mzdiff<- (findChromPeaks-centWave), 122
mzdiff<-,CentWaveParam-method (findChromPeaks-centWave), 122
mzdiff<-,MassifquantParam-method (findChromPeaks-massifquant), 133
mzdiff<-,MatchedFilterParam-method (findChromPeaks-matchedFilter), 140
mzIntervalExtension (findChromPeaks-centWaveWithPredIsoROIs), 128
mzIntervalExtension,CentWavePredIsoParam-method (findChromPeaks-centWaveWithPredIsoROIs), 128
mzIntervalExtension<- (findChromPeaks-centWaveWithPredIsoROIs), 128
mzIntervalExtension<-,CentWavePredIsoParam-method (findChromPeaks-centWaveWithPredIsoROIs), 128
mzR::writeMSData(), *287*
mzrange (xcmsEIC-class), 301
mzrange,xcmsEIC-method (xcmsEIC-class), 301
mzVsRtBalance (groupChromPeaks), 180
mzVsRtBalance,NearestPeaksParam-method (groupChromPeaks), 180
mzVsRtBalance<- (groupChromPeaks), 180
mzVsRtBalance<-,NearestPeaksParam-method (groupChromPeaks), 180

na.flatfill, 210
nearbyPeak (findPeaks-MSW), 152
nearbyPeak,MSWParam-method (findPeaks-MSW), 152
nearbyPeak<- (findPeaks-MSW), 152
nearbyPeak<-,MSWParam-method (findPeaks-MSW), 152
NearestPeaksParam (groupChromPeaks), 180
NearestPeaksParam-class (groupChromPeaks), 180
nls, *279*
noise (findChromPeaks-centWave), 122
noise,CentWaveParam-method (findChromPeaks-centWave), 122
noise,MassifquantParam-method (findChromPeaks-massifquant), 133
noise<- (findChromPeaks-centWave), 122

noise<-,CentWaveParam-method (findChromPeaks-centWave), 122
noise<-,MassifquantParam-method (findChromPeaks-massifquant), 133
normalize, *21, 22*
normalize,XCMSnExp-method (bin,XCMSnExp-method), 21
NumericList(), *257*

ObiwarpParam (adjustRtime), 7
ObiwarpParam-class (adjustRtime), 7
OnDiskMSnExp, *21–23*, *34*, *49*, *122*, *126, 127*, *129*, *132, 133*, *138–140*, *143, 144*, *152*, *155*, *202*, *206*, *305*, *314*, *327*
OnDiskMSnExp(), *12*, *118*
overlappingFeatures, 210, *314*
overlappingFeatures(), *111*

pairs, *212*
palette, *49*
panel.cor, 211
par(), *234*
Param (GenericParam-class), 171
Param-class (GenericParam-class), 171
pdf, *223*
PeakDensityParam, *229*
PeakDensityParam (groupChromPeaks), 180
PeakDensityParam(), *294*, *297*
PeakDensityParam-class (groupChromPeaks), 180
peakDetectionCWT, *68, 69*, *152*, *155*, *170, 171*
peakGroupsMatrix (adjustRtime), 7
peakGroupsMatrix,PeakGroupsParam-method (adjustRtime), 7
peakGroupsMatrix<- (adjustRtime), 7
peakGroupsMatrix<-,PeakGroupsParam-method (adjustRtime), 7
PeakGroupsParam (adjustRtime), 7
PeakGroupsParam-class (adjustRtime), 7
peakPlots,xcmsSet-method (peakPlots-methods), 212
peakPlots-methods, 212
peaks (xcmsSet-class), 323
peaks,xcmsSet-method (xcmsSet-class), 323
peaks<- (xcmsSet-class), 323
peaks<-,xcmsSet-method (xcmsSet-class), 323
peakScaleRange (findPeaks-MSW), 152
peakScaleRange,MSWParam-method (findPeaks-MSW), 152
peakScaleRange<- (findPeaks-MSW), 152
peakScaleRange<-,MSWParam-method (findPeaks-MSW), 152
peaksWithCentWave, *128*, 213, *216*
peaksWithCentWave(), *119, 120*
peaksWithMatchedFilter, *145*, *215*, 215
peaksWithMatchedFilter(), *121, 122*
peakTable (peakTable-methods), 217
peakTable,xcmsSet-method (peakTable-methods), 217
peakTable-methods, 217
peakThr (findPeaks-MSW), 152
peakThr,MSWParam-method (findPeaks-MSW), 152
peakThr<- (findPeaks-MSW), 152
peakThr<-,MSWParam-method (findPeaks-MSW), 152
peakwidth (findChromPeaks-centWave), 122
peakwidth,CentWaveParam-method (findChromPeaks-centWave), 122
peakwidth,MassifquantParam-method (findChromPeaks-massifquant), 133
peakwidth<- (findChromPeaks-centWave), 122
peakwidth<-,CentWaveParam-method (findChromPeaks-centWave), 122
peakwidth<-,MassifquantParam-method (findChromPeaks-massifquant), 133
PercentMissingFilter, *27, 28*, *76*, *115*, 218, *219*, *270, 271*
phenoData (xcmsSet-class), 323
phenoData,xcmsSet-method (xcmsSet-class), 323
phenoData<- (xcmsSet-class), 323
phenoData<-,xcmsSet,ANY-method (xcmsSet-class), 323
phenoData<-,xcmsSet-method (xcmsSet-class), 323
phenoDataFromPaths, 219
pickPeaks, *21, 22*
pickPeaks,XCMSnExp-method (bin,XCMSnExp-method), 21
PlainTextParam, 220, *221*, *255*, *281*

plot, *196*, *301*, *307*
plot(), *294*
plot, plot-methods *(*plot.xcmsEIC*)*, 222
plot,LamaParama,ANY-method *(*adjustRtime,XcmsExperiment,LamaParama-method*)*, 15
plot,MsExperiment,missing-method *(*filterFeatureDefinitions*)*, 99
plot,XChromatogram,ANY-method *(*XChromatograms*)*, 288
plot,XChromatograms,ANY-method *(*XChromatograms*)*, 288
plot,XCMSnExp,missing-method *(*XCMSnExp-class*)*, 305
plot.xcmsEIC, 222
plotAdjustedRtime, 223, *313*
plotAdjustedRtime(), *15*, *110, 111*
plotChrom, *233*, *248*, *320*
plotChrom *(*plotChrom-methods*)*, 225
plotChrom,xcmsRaw-method *(*plotChrom-methods*)*, 225
plotChrom-methods, 225
plotChromatogramsOverlay, 225
plotChromatogramsOverlay,MChromatograms-method *(*plotChromatogramsOverlay*)*, 225
plotChromatogramsOverlay,XChromatograms-method *(*plotChromatogramsOverlay*)*, 225
plotChromPeakDensity *(*plotChromPeakDensity,XCMSnExp-method*)*, 228
plotChromPeakDensity,XChromatograms-method *(*XChromatograms*)*, 288
plotChromPeakDensity,XCMSnExp-method, 228
plotChromPeakImage, *313*
plotChromPeakImage *(*plotChromPeaks*)*, 231
plotChromPeakImage(), *109*, *111*
plotChromPeaks, 231, *313*
plotChromPeaks(), *109*, *111*, *119*
plotEIC *(*plotEIC-methods*)*, 233
plotEIC,xcmsRaw-method *(*plotEIC-methods*)*, 233
plotEIC-methods, 233
plotFeatureGroups, 234
plotFeatureGroups(), *82*
plotMsData, 235
plotPeaks *(*plotPeaks-methods*)*, 236
plotPeaks,xcmsRaw-method *(*plotPeaks-methods*)*, 236
plotPeaks-methods, 236
plotQC, 236
plotRaw, *254*, *320*
plotRaw *(*plotRaw-methods*)*, 238
plotRaw,xcmsRaw-method *(*plotRaw-methods*)*, 238
plotRaw-methods, 238
plotrt, *325*
plotrt *(*plotrt-methods*)*, 238
plotrt,xcmsSet-method *(*plotrt-methods*)*, 238
plotrt-methods, 238
plotScan, *320*
plotScan *(*plotScan-methods*)*, 239
plotScan,xcmsRaw-method *(*plotScan-methods*)*, 239
plotScan-methods, 239
plotSpec, *248*, *320*
plotSpec *(*plotSpec-methods*)*, 240
plotSpec,xcmsRaw-method *(*plotSpec-methods*)*, 240
plotSpec-methods, 240
plotSurf, *320*
plotSurf *(*plotSurf-methods*)*, 240
plotSurf,xcmsRaw-method *(*plotSurf-methods*)*, 240
plotSurf-methods, 240
plotTIC, *320*
plotTIC *(*plotTIC-methods*)*, 241
plotTIC,xcmsRaw-method *(*plotTIC-methods*)*, 241
plotTIC-methods, 241
plotTree *(*xcmsFragments-class*)*, 304
plotTree,xcmsFragments-method *(*xcmsFragments-class*)*, 304
png, *223*
polarity,CentWavePredIsoParam-method *(*findChromPeaks-centWaveWithPredIsoROIs*)*, 128
polarity,MsExperiment-method *(*filterFeatureDefinitions*)*, 99
polarity<- *(*findChromPeaks-centWaveWithPredIsoROIs*)*, 128
polarity<-,CentWavePredIsoParam-method *(*findChromPeaks-centWaveWithPredIsoROIs*)*, 128

postscript, *223*
ppm *(*findChromPeaks-centWave*)*, 122
ppm,CentWaveParam-method *(*findChromPeaks-centWave*)*, 122
ppm,FillChromPeaksParam-method *(*fillChromPeaks*)*, 89
ppm,MassifquantParam-method *(*findChromPeaks-massifquant*)*, 133
ppm,MzClustParam-method *(*groupChromPeaks*)*, 180
ppm,PeakDensityParam-method *(*groupChromPeaks*)*, 180
ppm<- *(*findChromPeaks-centWave*)*, 122
ppm<-,CentWaveParam-method *(*findChromPeaks-centWave*)*, 122
ppm<-,FillChromPeaksParam-method *(*fillChromPeaks*)*, 89
ppm<-,MassifquantParam-method *(*findChromPeaks-massifquant*)*, 133
ppm<-,MzClustParam-method *(*groupChromPeaks*)*, 180
prefilter *(*findChromPeaks-centWave*)*, 122
prefilter,CentWaveParam-method *(*findChromPeaks-centWave*)*, 122
prefilter,MassifquantParam-method *(*findChromPeaks-massifquant*)*, 133
prefilter<- *(*findChromPeaks-centWave*)*, 122
prefilter<-,CentWaveParam-method *(*findChromPeaks-centWave*)*, 122
prefilter<-,MassifquantParam-method *(*findChromPeaks-massifquant*)*, 133
present *(*absent-methods*)*, 7
present,xcmsSet-method *(*absent-methods*)*, 7
processDate *(*ProcessHistory-class*)*, 242
processDate,ProcessHistory-method *(*ProcessHistory-class*)*, 242
ProcessHistory, *112*, *294*, *296*, *306*, *310*, *311*, *313*
ProcessHistory *(*ProcessHistory-class*)*, 242
processHistory, *171*, *305*
processHistory *(*XCMSnExp-class*)*, 305
processHistory(), *19*
processHistory,XChromatograms-method *(*XChromatograms*)*, 288
processHistory,XcmsExperiment-method *(*filterFeatureDefinitions*)*, 99
processHistory,XCMSnExp-method *(*XCMSnExp-class*)*, 305
ProcessHistory-class, 242
processHistoryTypes, *243*
processHistoryTypes *(*XCMSnExp-class*)*, 305
processHistoryTypes(), *106*
processInfo *(*ProcessHistory-class*)*, 242
processInfo,ProcessHistory-method *(*ProcessHistory-class*)*, 242
processParam *(*ProcessHistory-class*)*, 242
processParam,XProcessHistory-method *(*ProcessHistory-class*)*, 242
processType *(*ProcessHistory-class*)*, 242
processType,ProcessHistory-method *(*ProcessHistory-class*)*, 242
profBin, *248*, *322*, *323*
profBin *(*profGenerate*)*, 243
profBinLin, *322*
profBinLin *(*profGenerate*)*, 243
profBinLinBase, *322*
profBinLinBase *(*profGenerate*)*, 243
profBinLinBaseM *(*profGenerate*)*, 243
profBinLinM *(*profGenerate*)*, 243
profBinM *(*profGenerate*)*, 243
profGenerate, 243
profile-matrix, *8*
profile-matrix *(*profMat,MsExperiment-method*)*, 245
profinfo, *320*
profinfo *(*xcmsSet-class*)*, 323
profinfo,xcmsRaw-method *(*xcmsRaw-class*)*, 319
profinfo,xcmsSet-method *(*xcmsSet-class*)*, 323
profinfo<- *(*xcmsSet-class*)*, 323
profinfo<-,xcmsSet-method *(*xcmsSet-class*)*, 323
profIntLin, *322*
profIntLin *(*profGenerate*)*, 243
profIntLinM *(*profGenerate*)*, 243
profMat, *305*, *319*

profMat (profMat,MsExperiment-method), 245
profMat,MsExperiment-method, 245
profMat,OnDiskMSnExp-method (XCMSnExp-class), 305
profMat,XCMSnExp-method (XCMSnExp-class), 305
profMat,xcmsRaw-method (profMat,MsExperiment-method), 245
profMat-xcmsSet (profMat,MsExperiment-method), 245
profMaxIdx (profGenerate), 243
profMaxIdxM (profGenerate), 243
profMedFilt, *320*
profMedFilt (profMedFilt-methods), 248
profMedFilt,xcmsRaw-method (profMedFilt-methods), 248
profMedFilt-methods, 248
profMethod, *248*, *250*, *318*, *321*, *323*
profMethod (profMethod-methods), 248
profMethod,xcmsRaw-method (profMethod-methods), 248
profMethod,xcmsSet-method (xcmsSet-class), 323
profMethod-methods, 248
profMethod<-, *321*
profMethod<- (profMethod-methods), 248
profMethod<-,xcmsRaw-method (profMethod-methods), 248
profMz (xcmsRaw-class), 319
profMz,xcmsRaw-method (xcmsRaw-class), 319
profRange, *174*, *175*, *225*, *240*, *321*
profRange (profRange-methods), 249
profRange,xcmsRaw-method (profRange-methods), 249
profRange-methods, 249
profStep, *318*, *321*, *323*
profStep (profStep-methods), 250
profStep,xcmsRaw-method (profStep-methods), 250
profStep,xcmsSet-method (xcmsSet-class), 323
profStep-methods, 250
profStep<-, *321*
profStep<- (profStep-methods), 250
profStep<-,xcmsRaw-method (profStep-methods), 250
progressCallback (xcmsSet-class), 323
progressCallback,xcmsSet-method (xcmsSet-class), 323
progressCallback<- (xcmsSet-class), 323
progressCallback<-,xcmsSet-method (xcmsSet-class), 323
pSet, *314*
pval, 251

quantify, *314*
quantify,XcmsExperiment-method (filterFeatureDefinitions), 99
quantify,XCMSnExp-method, 251

rawEIC, *172*, *173*, *233*
rawEIC (rawEIC-methods), 253
rawEIC,xcmsRaw-method (rawEIC-methods), 253
rawEIC-methods, 253
rawMat (rawMat-methods), 254
rawMat,xcmsRaw-method (rawMat-methods), 254
rawMat-methods, 254
RDataParam, *221*, *255*, 255, *281*
reconstructChromPeakSpectra, 256
reconstructChromPeakSpectra(), *147*
reconstructChromPeakSpectra,XcmsExperiment-method (reconstructChromPeakSpectra), 256
reconstructChromPeakSpectra,XCMSnExp-method (reconstructChromPeakSpectra), 256
rectUnique, 258
refineChromPeaks, 259
refineChromPeaks(), *100*, *109*, *119*, *205*
refineChromPeaks,XChromatogram,MergeNeighboringPeaksParam-
(XChromatograms), 288
refineChromPeaks,XChromatograms,MergeNeighboringPeaksParam
(XChromatograms), 288
refineChromPeaks,XcmsExperiment,CleanPeaksParam-method (refineChromPeaks), 259
refineChromPeaks,XcmsExperiment,FilterIntensityParam-metho
(refineChromPeaks), 259
refineChromPeaks,XcmsExperiment,MergeNeighboringPeaksParam
(refineChromPeaks), 259
refineChromPeaks,XCMSnExp,CleanPeaksParam-method (refineChromPeaks), 259

refineChromPeaks,XCMSnExp,FilterIntensityParam-method (refineChromPeaks), 259
refineChromPeaks,XCMSnExp,MergeNeighboringPeaksParam-method (refineChromPeaks), 259
register, *127*, *132*, *139*, *144*, *155*
removeIntensity (removeIntensity,Chromatogram-method), 263
removeIntensity,Chromatogram-method, 263
removeIntensity,MChromatograms-method (removeIntensity,Chromatogram-method), 263
removeIntensity,XChromatogram-method (removeIntensity,Chromatogram-method), 263
removePeaks, *21*, *23*
removePeaks,XCMSnExp-method (bin,XCMSnExp-method), 21
response (adjustRtime), 7
response,ObiwarpParam-method (adjustRtime), 7
response<- (adjustRtime), 7
response<-,ObiwarpParam-method (adjustRtime), 7
retcor, *239*, *325*
retcor (retcor-methods), 265
retcor,xcmsSet-method (retcor-methods), 265
retcor-methods, 265
retcor.linear (retcor.peakgroups-methods), 267
retcor.linear,xcmsSet-method (retcor.peakgroups-methods), 267
retcor.loess, *265*
retcor.loess (retcor.peakgroups-methods), 267
retcor.loess,xcmsSet-method (retcor.peakgroups-methods), 267
retcor.obiwarp, *265*, 266, *267*
retcor.obiwarp,xcmsSet-method (retcor.obiwarp), 266
retcor.peakgroups (retcor.peakgroups-methods), 267
retcor.peakgroups,xcmsSet-method (retcor.peakgroups-methods), 267
retcor.peakgroups-methods, 267
retexp, 268
revMz (xcmsRaw-class), 319
revMz,xcmsRaw-method (xcmsRaw-class), 319
ridgeLength (findPeaks-MSW), 152
ridgeLength,MSWParam-method (findPeaks-MSW), 152
ridgeLength<- (findPeaks-MSW), 152
ridgeLength<-,MSWParam-method (findPeaks-MSW), 152
rla, 268
roiList (findChromPeaks-centWave), 122
roiList,CentWaveParam-method (findChromPeaks-centWave), 122
roiList<- (findChromPeaks-centWave), 122
roiList<-,CentWaveParam-method (findChromPeaks-centWave), 122
roiScales (findChromPeaks-centWave), 122
roiScales,CentWaveParam-method (findChromPeaks-centWave), 122
roiScales<- (findChromPeaks-centWave), 122
roiScales<-,CentWaveParam-method (findChromPeaks-centWave), 122
rowMax (colMax), 43
rowRla (rla), 268
RsdFilter, *27*, *28*, *76*, *115*, *219*, 269, *270*
rtime,MsExperiment-method (filterFeatureDefinitions), 99
rtime,XcmsExperiment-method (filterFeatureDefinitions), 99
rtime,XCMSnExp-method (XCMSnExp-class), 305
rtrange (xcmsEIC-class), 301
rtrange,xcmsEIC-method (xcmsEIC-class), 301

sampclass, *7*, *322*
sampclass (xcmsSet-class), 323
sampclass,xcmsSet-method (xcmsSet-class), 323
sampclass<- (xcmsSet-class), 323
sampclass<-,xcmsSet-method (xcmsSet-class), 323

sampleGroups (groupChromPeaks), 180
sampleGroups,MzClustParam-method (groupChromPeaks), 180
sampleGroups,NearestPeaksParam-method (groupChromPeaks), 180
sampleGroups,PeakDensityParam-method (groupChromPeaks), 180
sampleGroups<- (groupChromPeaks), 180
sampleGroups<-,MzClustParam-method (groupChromPeaks), 180
sampleGroups<-,NearestPeaksParam-method (groupChromPeaks), 180
sampleGroups<-,PeakDensityParam-method (groupChromPeaks), 180
sampnames, *301*, *325*
sampnames (sampnames-methods), 271
sampnames,xcmsEIC-method (sampnames-methods), 271
sampnames,xcmsSet-method (sampnames-methods), 271
sampnames-methods, 271
sampnames<- (xcmsSet-class), 323
sampnames<-,xcmsSet-method (xcmsSet-class), 323
scales (findPeaks-MSW), 152
scales,MSWParam-method (findPeaks-MSW), 152
scales<- (findPeaks-MSW), 152
scales<-,MSWParam-method (findPeaks-MSW), 152
scanrange (xcmsSet-class), 323
scanrange,xcmsRaw-method (xcmsRaw-class), 319
scanrange,xcmsSet-method (xcmsSet-class), 323
selfStart, *279*
SerialParam, *322*
setAs (XCMSnExp-class), 305
show, *304*
show,CleanPeaksParam-method (refineChromPeaks), 259
show,FilterIntensityParam-method (refineChromPeaks), 259
show,MergeNeighboringPeaksParam-method (refineChromPeaks), 259
show,MsFeatureData-method (XCMSnExp-class), 305
show,ProcessHistory-method (ProcessHistory-class), 242
show,XChromatogram-method (XChromatograms), 288
show,XChromatograms-method (XChromatograms), 288
show,xcmsEIC-method (xcmsEIC-class), 301
show,XcmsExperiment-method (filterFeatureDefinitions), 99
show,xcmsFragments-method (xcmsFragments-class), 304
show,XCMSnExp-method (XCMSnExp-class), 305
show,xcmsPeaks-method (xcmsPeaks-class), 316
show,xcmsRaw-method (xcmsRaw-class), 319
show,xcmsSet-method (xcmsSet-class), 323
show,XProcessHistory-method (ProcessHistory-class), 242
showError (showError,xcmsSet-method), 271
showError,xcmsSet-method, 271
sigma (findChromPeaks-matchedFilter), 140
sigma,MatchedFilterParam-method (findChromPeaks-matchedFilter), 140
sigma<- (findChromPeaks-matchedFilter), 140
sigma<-,MatchedFilterParam-method (findChromPeaks-matchedFilter), 140
SimilarRtimeParam(), *188*
smooth, *21*, *22*
smooth (adjustRtime), 7
smooth,PeakGroupsParam-method (adjustRtime), 7
smooth,XCMSnExp-method (bin,XCMSnExp-method), 21
smooth<- (adjustRtime), 7
smooth<-,PeakGroupsParam-method (adjustRtime), 7
SnowParam, *322*
SnowParam(), *283*
snthresh (findChromPeaks-centWave), 122
snthresh,CentWaveParam-method (findChromPeaks-centWave), 122
snthresh,MassifquantParam-method (findChromPeaks-massifquant),

133
snthresh,MatchedFilterParam-method (findChromPeaks-matchedFilter), 140
snthresh,MSWParam-method (findPeaks-MSW), 152
snthresh<- (findChromPeaks-centWave), 122
snthresh<-,CentWaveParam-method (findChromPeaks-centWave), 122
snthresh<-,MassifquantParam-method (findChromPeaks-massifquant), 133
snthresh<-,MatchedFilterParam-method (findChromPeaks-matchedFilter), 140
snthresh<-,MSWParam-method (findPeaks-MSW), 152
snthreshIsoROIs (findChromPeaks-centWaveWithPredIsoROIs), 128
snthreshIsoROIs,CentWavePredIsoParam-method (findChromPeaks-centWaveWithPredIsoROIs), 128
snthreshIsoROIs<- (findChromPeaks-centWaveWithPredIsoROIs), 128
snthreshIsoROIs<-,CentWavePredIsoParam-method (findChromPeaks-centWaveWithPredIsoROIs), 128
sortMz (xcmsRaw-class), 319
sortMz,xcmsRaw-method (xcmsRaw-class), 319
span (adjustRtime), 7
span,PeakGroupsParam-method (adjustRtime), 7
span<- (adjustRtime), 7
span<-,PeakGroupsParam-method (adjustRtime), 7
specDist (specDist-methods), 272
specDist,xcmsSet-method (specDist-methods), 272
specDist-methods, 272
specDist.cosine, 273
specDist.cosine,matrix,matrix-method (specDist.cosine), 273
specDist.meanMZmatch, 274
specDist.meanMZmatch,matrix,matrix-method (specDist.meanMZmatch), 274
specDist.peakCount (specDist.peakCount-methods), 275
specDist.peakCount,matrix,matrix-method (specDist.peakCount-methods), 275
specDist.peakCount-methods, 275
specNoise, 275, *277*
specPeaks, *276*, 276
Spectra, *39*
Spectra(), *86*, *87*, *110*, *118*, *257*
spectra,XCMSnExp-method (XCMSnExp-class), 305
spectrapply,XCMSnExp-method (XCMSnExp-class), 305
Spectrum, *40*, *306*, *313*
Spectrum2, *41*
split, *325*
split, split-methods (split.xcmsSet), 278
split,XCMSnExp,ANY-method ([,XCMSnExp,ANY,ANY,ANY-method), 327
split.screen, *212*, *236*
split.xcmsRaw, 277, *332*
split.xcmsSet, 278
SSgauss, 278
startup, *283*
steps (findChromPeaks-matchedFilter), 140
steps,MatchedFilterParam-method (findChromPeaks-matchedFilter), 140
steps<- (findChromPeaks-matchedFilter), 140
steps<-,MatchedFilterParam-method (findChromPeaks-matchedFilter), 140
stitch (stitch-methods), 279
stitch,xcmsRaw-method (stitch-methods), 279
stitch-methods, 279
stitch.netCDF (stitch-methods), 279
stitch.xml (stitch-methods), 279
storeResults, 281
storeResults,MsExperiment,PlainTextParam-method (PlainTextParam), 220

storeResults,XcmsExperiment,PlainTextParam-method (PlainTextParam), 220
storeResults,XcmsExperiment,RDataParam-method (RDataParam), 255
structure, *316*
subset (adjustRtime), 7
subset,ObiwarpParam-method (adjustRtime), 7
subset,PeakGroupsParam-method (adjustRtime), 7
subset-xcmsRaw ([,xcmsRaw,logicalOrNumeric,missing,missing-method), 332
subset<- (adjustRtime), 7
subset<-,ObiwarpParam-method (adjustRtime), 7
subset<-,PeakGroupsParam-method (adjustRtime), 7
subsetAdjust (adjustRtime), 7
subsetAdjust,ObiwarpParam-method (adjustRtime), 7
subsetAdjust,PeakGroupsParam-method (adjustRtime), 7
subsetAdjust<- (adjustRtime), 7
subsetAdjust<-,ObiwarpParam-method (adjustRtime), 7
subsetAdjust<-,PeakGroupsParam-method (adjustRtime), 7
SummarizedExperiment, *251*, *253*, *314*
SummarizedExperiment(), *111*
summarizeLamaMatch (adjustRtime,XcmsExperiment,LamaParama-method), 15

transformIntensity(), *296*
transformIntensity,XChromatogram-method (XChromatograms), 288
transformIntensity,XChromatograms-method (XChromatograms), 288
tuneIn (findPeaks-MSW), 152
tuneIn,MSWParam-method (findPeaks-MSW), 152
tuneIn<- (findPeaks-MSW), 152
tuneIn<-,MSWParam-method (findPeaks-MSW), 152
tuneInPeakInfo, *68*, *155*, *170*

unions (findChromPeaks-massifquant), 133
unions,MassifquantParam-method (findChromPeaks-massifquant), 133
unions<- (findChromPeaks-massifquant), 133
unions<-,MassifquantParam-method (findChromPeaks-massifquant), 133
uniqueMsLevels,MsExperiment-method (filterFeatureDefinitions), 99
updateObject,XCMSnExp-method (XCMSnExp-class), 305
updateObject,xcmsSet-method, 282
useOriginalCode, 282

vector, *316*
verboseColumns (findChromPeaks-centWave), 122
verboseColumns,CentWaveParam-method (findChromPeaks-centWave), 122
verboseColumns,MassifquantParam-method (findChromPeaks-massifquant), 133
verboseColumns,MSWParam-method (findPeaks-MSW), 152
verboseColumns<- (findChromPeaks-centWave), 122
verboseColumns<-,CentWaveParam-method (findChromPeaks-centWave), 122
verboseColumns<-,MassifquantParam-method (findChromPeaks-massifquant), 133
verboseColumns<-,MSWParam-method (findPeaks-MSW), 152
verify.mzQuantM, 283
verify.mzQuantML, *286*
verify.mzQuantML (verify.mzQuantM), 283

which.colMax (colMax), 43
which.rowMax (colMax), 43
withWave (findChromPeaks-massifquant), 133
withWave,MassifquantParam-method (findChromPeaks-massifquant), 133
withWave<- (findChromPeaks-massifquant), 133

withWave<-,MassifquantParam-method (findChromPeaks-massifquant), 133
write.cdf (write.cdf-methods), 284
write.cdf,xcmsRaw-method (write.cdf-methods), 284
write.cdf-methods, 284
write.mzdata (write.mzdata-methods), 285
write.mzdata,xcmsRaw-method (write.mzdata-methods), 285
write.mzdata-methods, 285
write.mzQuantML, *284*
write.mzQuantML (write.mzQuantML-methods), 285
write.mzQuantML,xcmsSet-method (write.mzQuantML-methods), 285
write.mzQuantML-methods, 285
writeMSData(), *287*
writeMSData,XCMSnExp,character-method, 286
writeMzTab, 287

XChromatogram, *120*
XChromatogram (XChromatograms), 288
XChromatogram(), *264*
XChromatogram-class (XChromatograms), 288
XChromatograms, *35*, *82*, 288
XChromatograms(), *37*, *83*, *84*, *97*, *98*, *108*, *226*, *264*, *330*
XChromatograms-class (XChromatograms), 288
xcms-deprecated, 300
xcmsEIC-class, 301
XcmsExperiment, *19*, *38*, *40*, *82*, *87*, *89*, *92*, *206*, *234*, *261*, *262*
XcmsExperiment (filterFeatureDefinitions), 99
XcmsExperiment(), *12*, *37*, *81*, *118*, *180*, *184–186*, *189*, *191*, *210*, *259*
XcmsExperiment-class (filterFeatureDefinitions), 99
xcmsFileSource, *326*
xcmsFileSource-class, 302
xcmsFragments, *42*, 303, *304*, *318*
xcmsFragments-class, 304
XCMSnExp, *19*, *21–23*, *31*, *32*, *34–36*, *38*, *40*, *49*, *79*, *81*, *82*, *87*, *100*, *127*, *128*, *132*, *133*, *139*, *144*, *145*, *155*, *156*, *171*, *193*, *206*, *229*, *252*, *253*, *261*, *286*, *307*, *327*, *329*, *330*
XCMSnExp (XCMSnExp-class), 305
XCMSnExp(), *12*, *81*, *112*, *118*, *180*, *184–186*, *189*, *191*, *210*, *234*, *259*, *295–297*
XCMSnExp-class, 305
XCMSnExp-filter ([,XCMSnExp,ANY,ANY,ANY-method), 327
xcmsPeaks-class, 316
xcmsRaw, *42*, *166–168*, *170*, *175*, *203*, *209*, *284*, *285*, *305*, *316*, 317, *319*, *321*, *326*, *327*, *332*
xcmsRaw-class, 319
xcmsSet, *42*, *127*, *132*, *139*, *144*, *155*, *166*, *237*, *271*, *282*, *286*, *287*, *304*, *305*, *314*, 321, *323–326*
xcmsSet-class, 323
xcmsSource, *204*, *302*, *327*
xcmsSource (xcmsSource-methods), 327
xcmsSource,character-method (xcmsFileSource-class), 302
xcmsSource,xcmsSource-method (xcmsSource-methods), 327
xcmsSource-class, 326
xcmsSource-methods, 327
xdata (loadXcmsData), 204
xmse (loadXcmsData), 204
XProcessHistory (ProcessHistory-class), 242
XProcessHistory-class (ProcessHistory-class), 242