Package 'flagme'

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Title Analysis of Metabolomics GC/MS Data

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Imports gplots, graphics, MASS, methods, SparseM, stats, utils

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Contents

addAMDISPeaks *Add AMDIS peak detection results*

Description

Reads ASCII ELU-format files (output from AMDIS) and attaches them to an already created peaksDataset object

Usage

```
addAMDISPeaks(object, fns = dir(, "[Eu][Ll][Uu]"), verbose = TRUE, ...)
```

Arguments

object	a peaksDataset object.
fns	character vector of same length as object@rawdata (user ensures the order matches)
verbose	whether to give verbose output, default TRUE
...	arguments passed on to parseELU

Details

Repeated calls to parseELU to add peak detection results to the original peaksDataset object.

Value

peaksDataset object

Author(s)

Mark Robinson

References

Mark D Robinson (2008). Methods for the analysis of gas chromatography - mass spectrometry data *PhD dissertation* University of Melbourne.

See Also

parseELU, peaksDataset

Examples

```
# need access to CDF (raw data) and ELU files
require(gcspikelite)
gcmsPath<-paste(find.package("gcspikelite"),"data",sep="/")

# full paths to file names
cdfFiles<-dir(gcmsPath,"CDF",full=TRUE)
eluFiles<-dir(gcmsPath,"ELU",full=TRUE)

# create a 'peaksDataset' object and add AMDIS peaks to it
pd<-peaksDataset(cdfFiles[1],mz=seq(50,550),rtrange=c(7.5,8.5))
pd<-addAMDISPeaks(pd,eluFiles[1])
```

---

addChromaTOFPeaks *Add ChromaTOF peak detection results*

Description

Reads ASCII tab-delimited format files (output from ChromaTOF) and attaches them to an already created `peaksDataset` object

Usage

```
addChromaTOFPeaks(
  object,
  fns = dir(, "[Tt][Xx][Tx]"),
  rtDivide = 60,
  verbose = TRUE,
  ...
)
```

Arguments

`object`	a `peaksDataset` object.
`fns`	character vector of same length as `object@rawdata` (user ensures the order matches)
`rtDivide`	number giving the amount to divide the retention times by.
`verbose`	whether to give verbose output, default `TRUE`
`...`	arguments passed on to `parseChromaTOF`

Details

Repeated calls to `parseChromaTOF` to add peak detection results to the original `peaksDataset` object.

Value

peaksDataset object

Author(s)

Mark Robinson

References

Mark D Robinson (2008). Methods for the analysis of gas chromatography - mass spectrometry data *PhD dissertation* University of Melbourne.

See Also

parseChromaTOF, peaksDataset

Examples

```
# need access to CDF (raw data) and ChromaTOF files
require(gcspikelite)
gcmsPath<-paste(find.package("gcspikelite"),"data",sep="/")

# full paths to file names
cdfFiles<-dir(gcmsPath,"CDF",full=TRUE)
# [not run] cTofFiles<-dir(gcmsPath,"txt",full=TRUE)

# create a 'peaksDataset' object and add ChromaTOF peaks to it
pd<-peaksDataset(cdfFiles[1],mz=seq(50,550),rtrange=c(7.5,8.5))
# [not run] pd<-addChromTOFPeaks(pd,...)
```

---

addXCMSPeaks *addXCMSPeaks*

Description

Add xcms/CAMERA peak detection results

Usage

```
addXCMSPeaks(
  files,
  object,
  settings = list(),
  minintens = 100,
  minfeat = 6,
  BPPARAM = bpparam(),
  multipleMF = FALSE,
  multipleMFParam = list(fwhm = c(5, 10, 15), mz.abs = 0.2, rt.abs = 2)
)
```

Arguments

files	list of chromatogram files
object	a peakDataset object
settings	see findPeaks-matchedFilter findPeaks-centWave
minintens	minimum ion intensity to be included into a pseudospectra
minfeat	minimum number of ion to be created a pseudospectra
BPPARAM	a parameter class specifying if and how parallel processing should be performed
multipleMF	logical Try to remove redundant peaks, in this case where there are any peaks within an absolute m/z value of 0.2 and within 3 s for any one sample in the xcmsSet (the largest peak is kept)
multipleMFParam	list. It conteins the settings for the peak-picking. mz_abs represent the the mz range; rt_abs represent thert range
mz.abs	mz range
rt.abs	rt range

Details

Reads the raw data using xcms, group each extracted ion according to their retention time using CAMERA and attaches them to an already created peaksDataset object

Repeated calls to xcmsSet and annotate to perform peak-picking and deconvolution. The peak detection results are added to the original peaksDataset object. Two peak detection alorithms are available: continuous wavelet transform (peakPicking=c('cwt')) and the matched filter approach (peakPicking=c('mF')) described by Smith et al (2006). For further information consult the xcms package manual.

Value

peaksDataset object

Author(s)

Riccardo Romoli <riccardo.romoli@unifi.it>

See Also

peaksDataset findPeaks-matchedFilter findPeaks-centWave xcmsRaw-class

Examples

```
files <- list.files(path = paste(find.package("gcspikelite"), "data",
                    sep = "/"),"CDF", full = TRUE)
data <- peaksDataset(files[1:2], mz = seq(50, 550), rtrange = c(7.5, 8.5))
## create settings object
mfp <- xcms::MatchedFilterParam(fwhm = 10, snthresh = 5)
cwt <- xcms::CentWaveParam()
data <- addXCMSPeaks(files[1:2], data, settings = mfp, multipleMF = FALSE)
data
```

betweenAlignment *Data Structure for "between" alignment of many GCMS samples*

Description

This function creates a "between" alignment (i.e. comparing merged peaks)

Usage

```
betweenAlignment(
  pD,
  cAList,
  pAList,
  impList,
  filterMin = 1,
  gap = 0.7,
  D = 10,
  usePeaks = TRUE,
  df = 30,
  verbose = TRUE,
  metric = 2,
  type = 2,
  penality = 0.2,
  compress = FALSE
)
```

Arguments

pD	a peaksDataset object
cAList	list of clusterAlignment objects, one for each experimental group
pAList	list of progressiveAlignment objects, one for each experimental group
impList	list of imputation lists
filterMin	minimum number of peaks within a merged peak to be kept in the analysis
gap	gap parameter
D	retention time penalty parameter
usePeaks	logical, whether to use peaks (if TRUE) or the full 2D profile alignment (if FALSE)
df	distance from diagonal to calculate similarity
verbose	logical, whether to print information
metric	numeric, different algorithm to calculate the similarity matrix between two mass spectrum. metric=1 call normDotProduct(); metric=2 call ndpRT(); metric=3 call corPrt()
type	numeric, two different type of alignment function
penality	penalization applied to the matching between two mass spectra if (t1-t2)>D
compress	logical whether to compress the similarity matrix into a sparse format.

Details

betweenAlignment objects gives the data structure which stores the result of an alignment across several "pseudo" datasets. These pseudo datasets are constructed by merging the "within" alignments.

Value

betweenAlignment object

Author(s)

Mark Robinson

References

Mark D Robinson (2008). Methods for the analysis of gas chromatography - mass spectrometry data *PhD dissertation* University of Melbourne.

See Also

multipleAlignment

Examples

```
require(gcspikelite)
## see 'multipleAlignment'
```

---

calcTimeDiffs *Calculate retention time shifts from profile alignments*

Description

This function takes the set of all pairwise profile alignments and use these to estimate retention time shifts between each pair of samples. These will then be used to normalize the retention time penalty of the signal peak alignment.

Usage

```
calcTimeDiffs(pd, ca.full, verbose = TRUE)
```

Arguments

pd	a peaksDataset object
ca.full	a clusterAlignment object, fit with
verbose	logical, whether to print out information

Details

Using the set of profile alignments,

Value

`list` of same length as `ca.full@alignments` with the matrices giving the retention time penalties.

Author(s)

Mark Robinson

References

Mark D Robinson (2008). Methods for the analysis of gas chromatography - mass spectrometry data *PhD dissertation* University of Melbourne.

See Also

`peaksAlignment`, `clusterAlignment`

Examples

```
require(gcspikelite)

# paths and files
gcmsPath <- paste(find.package("gcspikelite"),"data",sep="/")
cdfFiles <- dir(gcmsPath,"CDF",full=TRUE)
eluFiles <- dir(gcmsPath,"ELU",full=TRUE)

# read data, peak detection results
pd <- peaksDataset(cdfFiles[1:2],mz=seq(50,550),rtrange=c(7.5,8.5))
pd <- addAMDISPeaks(pd,eluFiles[1:2])

# pairwise alignment using all scans
fullca <- clusterAlignment(pd, usePeaks=FALSE, df=100)

# calculate retention time shifts
timedf <- calcTimeDiffs(pd, fullca)
```

---

clusterAlignment *Data Structure for a collection of all pairwise alignments of GCMS runs*

Description

Store the raw data and optionally, information regarding signal peaks for a number of GCMS runs

Usage

```
clusterAlignment(
  pD,
  runs = 1:length(pD@rawdata),
  timedf = NULL,
  usePeaks = TRUE,
  verbose = TRUE,
  ...
)
```

Arguments

pD	a peaksDataset object.
runs	vector of integers giving the samples to calculate set of pairwise alignments over.
timedf	list (length = the number of pairwise alignments) of matrices giving the expected time differences expected at each pair of peaks used with usePeaks=TRUE, passed to peaksAlignment
usePeaks	logical, TRUE uses peakdata list, FALSE uses rawdata list for computing similarity.
verbose	logical, whether to print out info.
...	other arguments passed to peaksAlignment

Details

clusterAlignment computes the set of pairwise alignments.

Value

clusterAlignment object

Author(s)

Mark Robinson, Riccardo Romoli

References

Mark D Robinson (2008). Methods for the analysis of gas chromatography - mass spectrometry data *PhD dissertation* University of Melbourne.

See Also

peaksDataset, peaksAlignment

Examples

```
require(gcspikelite)

# paths and files
gcmsPath <- paste(find.package("gcspikelite"), "data", sep="/")
cdfFiles <- dir(gcmsPath, "CDF", full=TRUE)
eluFiles <- dir(gcmsPath, "ELU", full=TRUE)

# read data, peak detection results
pd <- peaksDataset(cdfFiles[1:2], mz=seq(50,550), rtrange=c(7.5,8.5))
pd <- addAMDISPeaks(pd, eluFiles[1:2])

ca <- clusterAlignment(pd, gap=0.5, D=0.05, df=30, metric=1, type=1)
```

---

compress,peaksAlignment-method

Compression method for peaksAlignment object

Description

Compression method for peaksAlignment object

Usage

```
## S4 method for signature 'peaksAlignment'
compress(object, verbose = TRUE, ...)
```

Arguments

object	peaksAlignment
verbose	logical
...	further

Author(s)

MR

compress,progressiveAlignment-method *Compress method for progressiveAlignment*

Description

Decompress method for progressiveAlignment

Usage

```
## S4 method for signature 'progressiveAlignment'
compress(object, verbose = TRUE, ...)
```

Arguments

object	dummy
verbose	dummy
...	dummy

Details

Deompress method for progressiveAlignment

Author(s)

MR

corPrt *Retention Time Penalized Correlation*

Description

This function calculates the similarity of all pairs of peaks from 2 samples, using the spectra similarity and the rretention time differencies

Usage

```
corPrt(d1, d2, t1, t2, D, penality = 0.2)
```

Arguments

d1	data matrix for sample 1
d2	data matrix for sample 2
t1	vector of retention times for sample 1
t2	vector of retention times for sample 2
D	retention time window for the matching
penality	penalization applied to the matching between two mass spectra if (t1-t2)>D

Details

Computes the Pearson carrelation between every pair of peak vectors in the retention time window (D)and returns the similarity matrix.

Value

matrix of similarities

Author(s)

Riccardo Romoli

See Also

peaksAlignment

Examples

```
## Not Run
require(gcspikelite)
files <- list.files(path = paste(find.package("gcspikelite"), "data",
                    sep = "/"),"CDF", full = TRUE)
data <- peaksDataset(files[1:2], mz = seq(50, 550), rtrange = c(7.5, 8.5))
## create settings object
mfp <- xcms::MatchedFilterParam(fwhm = 10, snthresh = 5)
cwt <- xcms::CentWaveParam()
data <- addXCMSPeaks(files[1:2], data, settings = mfp, multipleMF = FALSE)
data
## review peak picking
plotChrom(data, rtrange=c(7.5, 10.5), runs=c(1:2))

r <- corPrt(data@peaksdata[[1]], data@peaksdata[[2]],
          data@peaksrt[[1]], data@peaksrt[[2]], D = 50, penality = 0.2)
## End (Not Run)
```

---

decompress,peaksAlignment-method

Decompression method for peaksAlignment object

Description

Decompression method for peaksAlignment object

Usage

```
## S4 method for signature 'peaksAlignment'
decompress(object, verbose = TRUE, ...)
```

Arguments

object	peaksAlignment object
verbose	dummy
...	dummy

Author(s)

MR

---

decompress,progressiveAlignment-method

Compress method for progressiveAlignment

Description

Decompress method for progressiveAlignment

Usage

```
## S4 method for signature 'progressiveAlignment'
decompress(object, verbose = TRUE, ...)
```

Arguments

object	progressiveAlignment object
verbose	logical
...	dummy

Details

Decompress method for progressiveAlignment

Author(s)

MR

deDuper *deDuper*

Description

Duplicate peak removal function

Usage

```
deDuper(object, mz.abs = 0.1, rt.abs = 2)
```

Arguments

object	xcms object
mz.abs	mz range
rt.abs	rt range

Details

Remove redundant peaks, in this case where there are any peaks within an absolute m/z value of 0.2 and within 3 s for any one sample in the xcmsSet (the largest peak is kept)

Value

an object of xcms class

Author(s)

r

---

distToLib *distToLib*

Description

The function calculate the distance between each mas spec in the msp file and the aligned mass spec from each sampe

Usage

```
distToLib(mspLib, outList)
```

Arguments

mspLib	a .msp file from NIST
outList	an object from gatherInfo()

Details

Return the distance matrix

Value

the distance matrix between the mass spec and the aligned spec

Author(s)

Riccardo Romoli

`dp` *Dynamic programming algorithm, given a similarity matrix*

Description

This function calls C code for a bare-bones dynamic programming algorithm, finding the best cost path through a similarity matrix.

Usage

```
dp(M, gap = 0.5, big = 1e+10, verbose = FALSE)
```

Arguments

`M`	similarity matrix
`gap`	penalty for gaps
`big`	large value used for matrix margins
`verbose`	logical, whether to print out information

Details

This is a pretty standard implementation of a bare-bones dynamic programming algorithm, with a single gap parameter and allowing only simple jumps through the matrix (up, right or diagonal).

Value

`list` with element `match` with the set of pairwise matches.

Author(s)

Mark Robinson

References

Mark D Robinson (2008). Methods for the analysis of gas chromatography - mass spectrometry data *PhD dissertation* University of Melbourne.

See Also

normDotProduct

Examples

```
require(gcspikelite)

# paths and files
gcmsPath<-paste(find.package("gcspikelite"),"data",sep="/")
cdfFiles<-dir(gcmsPath,"CDF",full=TRUE)
eluFiles<-dir(gcmsPath,"ELU",full=TRUE)

# read data, peak detection results
pd<-peaksDataset(cdfFiles[1:2],mz=seq(50,550),rtrange=c(7.5,8.5))
pd<-addAMDISPeaks(pd,eluFiles[1:2])

# similarity matrix
r<-normDotProduct(pd@peaksdata[[1]],pd@peaksdata[[2]])

# dynamic-programming-based matching of peaks
v<-dp(r,gap=.5)
```

---

dynRT *dynRT*

Description

Dynamic Retention Time Based Alignment algorithm, given a similarity matrix

Usage

```
dynRT(S)
```

Arguments

S	similarity matrix

Details

This function align two chromatograms finding the maximum similarity among the mass spectra

Value

list containing the matched peaks between the two chromatograms. The number represent position of the spectra in the S matrix

Author(s)

riccardo.romoli@unifi.it

Examples

```
require(gcspikelite)
files <- list.files(path = paste(find.package("gcspikelite"), "data",
                    sep = "/"),"CDF", full = TRUE)
data <- peaksDataset(files[1:2], mz = seq(50, 550), rtrange = c(7.5, 8.5))
## create settings object
mfp <- xcms::MatchedFilterParam(fwhm = 10, snthresh = 5)
cwt <- xcms::CentWaveParam()
data <- addXCMSPeaks(files[1:2], data, settings = mfp, multipleMF = FALSE)
data
## review peak picking
plotChrom(data, rtrange=c(7.5, 10.5), runs=c(1:2))
## similarity
r <- ndpRT(data@peaksdata[[1]], data@peaksdata[[2]], data@peaksrt[[1]],
    data@peaksrt[[2]], D = 50)
## dynamic retention time based alignment algorithm
v <- dynRT(S = r)
```

`eitherMatrix-class` *A class description*

Description

A class description

`exportSpectra` *exportSpectra*

Description

Write the mass spectum into a .msp file to be used in NIST search.

Usage

```
exportSpectra(object, outList, spectra, normalize = TRUE)
```

Arguments

`object`	an object of class "peaksDataset"
`outList`	an object created using the gatherInfo() function
`spectra`	numeric. The number of the mass spectra to be printed. It correspond to the number of the peak in the plot() and the number of the peak in the gatherInfo() list.
`normalize`	logical. If the mass spectra has to be normalized to 100

Details

Write the mass spectum into a .msp file to be used in NIST search.

Value

a .msp file

Author(s)

riccardo.romoli@unifi.com

`gatherInfo` *Gathers abundance informations from an alignment*

Description

Given an alignment table (indices of matched peaks across several samples) such as that within a `progressiveAlignment` or `multipleAlignment` object, this routines goes through the raw data and collects the abundance of each fragment peak, as well as the retention times across the samples.

Usage

```
gatherInfo(
  pD,
  obj,
  newind = NULL,
  method = c("apex"),
  findmzind = TRUE,
  useTIC = FALSE,
  top = NULL,
  intensity.cut = 0.05
)
```

Arguments

`pD`	a `peaksDataset` object, to get the abundance data from
`obj`	either a `multipleAlignment` or `progressiveAlignment` object
`newind`	list giving the
`method`	method used to gather abundance information, only `apex` implemented currently.
`findmzind`	logical, whether to take a subset of all m/z indices
`useTIC`	logical, whether to use total ion current for abundance summaries
`top`	only use the top `top` peaks
`intensity.cut`	percentage of the maximum intensity

Details

This procedure loops through the the table of matched peaks and gathers the

Value

Returns a list (of lists) for each row in the alignment table. Each list has 3 elements:

`mz`	a numerical vector of the m/z fragments used
`rt`	a numerical vector for the exact retention time of each peak across all samples
`data`	matrix of fragment intensities. If `useTIC = TRUE`, this matrix will have a single row

Author(s)

Mark Robinson

References

Mark D Robinson (2008). Methods for the analysis of gas chromatography - mass spectrometry data *PhD dissertation* University of Melbourne.

See Also

`imputePeaks`

Examples

```
require(gcspikelite)

## paths and files
gcmsPath <- paste(find.package("gcspikelite"), "data", sep = "/")
cdfFiles <- dir(gcmsPath, "CDF", full = TRUE)
eluFiles <- dir(gcmsPath, "ELU", full = TRUE)

## read data, peak detection results
pd <- peaksDataset(cdfFiles[1:2], mz = seq(50, 550), rtrange = c(7.5, 8.5))
pd <- addAMDISPeaks(pd, eluFiles[1:2])

## multiple alignment
ma <- multipleAlignment(pd, c(1,1), wn.gap = 0.5, wn.D = 0.05, bw.gap = 0.6,
                        bw.D = 0.2, usePeaks = TRUE, filterMin = 1, df = 50,
                        verbose = TRUE, metric = 1, type = 1)

## gather apex intensities
d <- gatherInfo(pd, ma)

## table of retention times
nm <- list(paste("MP", 1:length(d), sep = ""), c("S1", "S2"))
rts <- matrix(unlist(sapply(d, .subset, "rt")), byrow = TRUE, nc = 2,
              dimnames = nm)
```

headToTailPlot *Head to tail plot*

Description

The head-to-tail-plot for the mass spectra

Usage

```
headToTailPlot(specFromLib, specFromList)
```

Arguments

specFromLib	the mass spectra obtained from the .msp file
specFromList	the mass spectra obtained from gatherInfo

Details

Head-to-tail-plot to visually compare the mass spectra

Value

the plot

Author(s)

Riccardo Romoli

importSpec *importSpec*

Description

Read the mass spectra from an external msp file

Usage

```
importSpec(file)
```

Arguments

file	a .msp file from NIST search library database

Details

Read the mass spectra from an external file in msp format. The format is used in NIST search library database.

Value

list conaining the mass spctra

Author(s)

riccardo.romoli@unifi.it

`imputePeaks` *Imputatin of locations of peaks that were undetected*

Description

Using the information within the peaks that are matched across several runs, we can impute the location of the peaks that are undetected in a subset of runs

Usage

```
imputePeaks(pD, obj, typ = 1, obj2 = NULL, filterMin = 1, verbose = TRUE)
```

Arguments

`pD`	a `peaksDataset` object
`obj`	the alignment object, either `multipleAlignment` or `progressiveAlignment`, that is used to infer the unmatched peak locations
`typ`	type of imputation to do, 1 for simple linear interpolation (default), 2 only works if `obj2` is a `clusterAlignment` object
`obj2`	a `clusterAlignment` object
`filterMin`	minimum number of peaks within a merged peak to impute
`verbose`	logical, whether to print out information

Details

If you are aligning several samples and for a (small) subset of the samples in question, a peak is undetected, there is information within the alignment that can be useful in determining where the undetected peak is, based on the surrounding matched peaks. Instead of moving forward with missing values into the data matrices, this procedures goes back to the raw data and imputes the location of the apex (as well as the start and end), so that we do not need to bother with post-hoc imputation or removing data because of missing components.

We realize that imputation is prone to error and prone to attributing intensity from neighbouring peaks to the unmatched peak. We argue that this is still better than having to deal with these in statistical models after that fact. This may be an area of future improvement.

Value

`list` with 3 elements `apex`, `start` and `end`, each masked matrices giving the scan numbers of the imputed peaks.

Author(s)

Mark Robinson

References

Mark D Robinson (2008). Methods for the analysis of gas chromatography - mass spectrometry data *PhD dissertation* University of Melbourne.

See Also

multipleAlignment, progressiveAlignment, peaksDataset

Examples

```
require(gcspikelite)

## paths and files
gcmsPath <- paste(find.package("gcspikelite"), "data", sep = "/")
cdfFiles <- dir(gcmsPath,"CDF", full = TRUE)
eluFiles <- dir(gcmsPath,"ELU", full = TRUE)

## read data, peak detection results
pd <- peaksDataset(cdfFiles[1:3], mz = seq(50,550), rtrange = c(7.5,8.5))
pd <- addAMDISPeaks(pd, eluFiles[1:3])

## alignments
ca <- clusterAlignment(pd, gap = 0.5, D = 0.05, df = 30, metric = 1, type =
   1, compress = FALSE)
pa <-progressiveAlignment(pd, ca, gap = 0.6, D = 0.1, df = 30,
                          compress = FALSE)

v <- imputePeaks(pd, pa, filterMin = 1)
```

---

matchSpec *matchSpec*

Description

Calculate the distance between a reference mass spectrum

Usage

```
matchSpec(spec1, outList, whichSpec)
```

Arguments

spec1	reference mass spectrum
outList	the return of gatherInfo
whichSpec	the entry number of outList

Details

Calculate the distance between a reference mass spectrum and one from the sample

Value

the distance between the reference mass spectrum and the others

Author(s)

Riccardo Romoli

`multipleAlignment-class` *Data Structure for multiple alignment of many GCMS samples*

Description

Store the raw data and optionally, information regarding signal peaks for a number of GCMS runs

Usage

```
multipleAlignment(
  pd,
  group,
  bw.gap = 0.8,
  wn.gap = 0.6,
  bw.D = 0.2,
  wn.D = 0.05,
  filterMin = 1,
  lite = FALSE,
  usePeaks = TRUE,
  df = 50,
  verbose = TRUE,
  timeAdjust = FALSE,
  doImpute = FALSE,
  metric = 2,
  type = 2,
  penality = 0.2,
  compress = FALSE
)
```

Arguments

`pd`	a `peaksDataset` object
`group`	factor variable of experiment groups, used to guide the alignment algorithm
`bw.gap`	gap parameter for "between" alignments

wn.gap	gap parameter for "within" alignments
bw.D	distance penalty for "between" alignments. When type = 2 represent the retention time window expressed in seconds
wn.D	distance penalty for "within" alignments. When type = 2 represent the retention time window expressed in seconds
filterMin	minimum number of peaks within a merged peak to be kept in the analysis
lite	logical, whether to keep "between" alignment details (default, FALSE)
usePeaks	logical, whether to use peaks (if TRUE) or the full 2D profile alignment (if FALSE)
df	distance from diagonal to calculate similarity
verbose	logical, whether to print information
timeAdjust	logical, whether to use the full 2D profile data to estimate retention time drifts (Note: time required)
doImpute	logical, whether to impute the location of unmatched peaks
metric	numeric, different algorithm to calculate the similarity matrix between two mass spectrum. metric=1 call normDotProduct(); metric=2 call ndpRT(); metric=3 call corPrt()
type	numeric, two different type of alignment function
penality	penalization applied to the matching between two mass spectra if (t1-t2)>D
compress	logical whether to compress the similarity matrix into a sparse format.

Details

multipleAlignment is the data structure giving the result of an alignment across several GCMS runs. Multiple alignments are done progressively. First, all samples with the same tg$Group label with be aligned (denoted a "within" alignment). Second, each group will be summarized into a pseudo-data set, essentially a spectrum and retention time for each matched peak of the within-alignment. Third, these "merged peaks" are aligned in the same progressive manner, here called a "between" alignment.

Value

multipleAlignment object

Author(s)

Mark Robinson

References

Mark D Robinson (2008). Methods for the analysis of gas chromatography - mass spectrometry data *PhD dissertation* University of Melbourne.

See Also

peaksDataset, betweenAlignment, progressiveAlignment

Examples

```
 require(gcspikelite)

## paths and files
gcmsPath <- paste(find.package("gcspikelite"), "data", sep = "/")
cdfFiles <- dir(gcmsPath, "CDF", full = TRUE)
eluFiles <- dir(gcmsPath, "ELU", full = TRUE)

## read data, peak detection results
pd <- peaksDataset(cdfFiles[1:2], mz = seq(50, 550), rtrange = c(7.5, 8.5))
pd <- addAMDISPeaks(pd,eluFiles[1:2])

## multiple alignment
ma <- multipleAlignment(pd, c(1, 1), wn.gap = 0.5, wn.D = 0.05, bw.gap = 0.6,
                        bw.D = 0.2, usePeaks = TRUE, filterMin = 1, df = 50,
                        verbose = TRUE, metric = 1, type = 1)
```

---

ndpRT *Retention Time Penalized Normalized Dot Product*

Description

This function calculates the similarity of all pairs of peaks from 2 samples, using the spectra similarity and the retention time differencies

Usage

```
ndpRT(s1, s2, t1, t2, D)
```

Arguments

s1	data matrix for sample 1
s2	data matrix for sample 2
t1	vector of retention times for sample 1
t2	vector of retention times for sample 2
D	retention time window for the matching

Details

Computes the normalized dot product between every pair of peak vectors in the retention time window (D)and returns a similarity matrix.

Value

matrix of similarities

Author(s)

Riccardo Romoli

See Also

peaksAlignment

Examples

```
## Not Run
require(gcspikelite)
files <- list.files(path = paste(find.package("gcspikelite"), "data",
                    sep = "/"),"CDF", full = TRUE)
data <- peaksDataset(files[1:2], mz = seq(50, 550), rtrange = c(7.5, 8.5))
## create settings object
mfp <- xcms::MatchedFilterParam(fwhm = 10, snthresh = 5)
cwt <- xcms::CentWaveParam()
data <- addXCMSPeaks(files[1:2], data, settings = mfp, multipleMF = FALSE)
data
## review peak picking
plotChrom(data, rtrange = c(7.5, 10.5), runs = c(1:2))

r <- ndpRT(data@peaksdata[[1]], data@peaksdata[[2]],
           data@peaksrt[[1]], data@peaksrt[[2]], D = 50)
## End (Not Run)
```

---

normDotProduct *Normalized Dot Product*

Description

This function calculates the similarity of all pairs of peaks from 2 samples, using the spectra similarity

Usage

```
normDotProduct(
  x1,
  x2,
  t1 = NULL,
  t2 = NULL,
  df = max(ncol(x1), ncol(x2)),
  D = 1e+05,
  timedf = NULL,
  verbose = FALSE
)
```

Arguments

x1	data matrix for sample 1
x2	data matrix for sample 2
t1	vector of retention times for sample 1
t2	vector of retention times for sample 2
df	distance from diagonal to calculate similarity
D	retention time penalty
timedf	matrix of time differences to normalize to. if NULL, 0 is used.
verbose	logical, whether to print out information

Details

Efficiently computes the normalized dot product between every pair of peak vectors and returns a similarity matrix. C code is called.

Value

matrix of similarities

Author(s)

Mark Robinson

References

Mark D Robinson (2008). Methods for the analysis of gas chromatography - mass spectrometry data *PhD dissertation* University of Melbourne.

See Also

dp, peaksAlignment

Examples

```
require(gcspikelite)

# paths and files
gcmsPath<-paste(find.package("gcspikelite"),"data",sep="/")
cdfFiles<-dir(gcmsPath,"CDF",full=TRUE)
eluFiles<-dir(gcmsPath,"ELU",full=TRUE)

# read data, peak detection results
pd<-peaksDataset(cdfFiles[1:2],mz=seq(50,550),rtrange=c(7.5,8.5))
pd<-addAMDISPeaks(pd,eluFiles[1:2])

r<-normDotProduct(pd@peaksdata[[1]],pd@peaksdata[[2]])
```

parseChromaTOF *Parser for ChromaTOF files*

Description

Reads ASCII ChromaTOF-format files from AMDIS (Automated Mass Spectral Deconvolution and Identification System)

Usage

```
parseChromaTOF(
  fn,
  min.pc = 0.01,
  mz = seq(85, 500),
  rt.cut = 0.008,
  rtrange = NULL,
  skip = 1,
  rtDivide = 60
)
```

Arguments

fn	ChromaTOF filename to read.
min.pc	minimum percent of maximum intensity.
mz	vector of mass-to-charge bins of raw data table.
rt.cut	the difference in retention time, below which peaks are merged together.
rtrange	retention time range to parse peaks from, can speed up parsing if only interested in a small region (must be numeric vector of length 2)
skip	number of rows to skip at beginning of the ChromaTOF
rtDivide	multiplier to divide the retention times by (default: 60)

Details

parseChromaTOF will typically be called by addChromaTOFPeaks, not called directly.

Peaks that are detected within rt.cut are merged together. This avoids peaks which are essentially overlapping.

Fragments that are less than min.pc of the maximum intensity fragment are discarded.

Value

list with components peaks (table of spectra – rows are mass-to-charge and columns are the different detected peaks) and tab (table of features for each detection), according to what is stored in the ChromaTOF file.

Author(s)

Mark Robinson

References

Mark D Robinson (2008). Methods for the analysis of gas chromatography - mass spectrometry data *PhD dissertation* University of Melbourne.

See Also

addAMDISPeaks

Examples

```
require(gcspikelite)

# paths and files
gcmsPath<-paste(find.package("gcspikelite"),"data",sep="/")
tofFiles<-dir(gcmsPath,"tof",full=TRUE)

# parse ChromaTOF file
cTofList<-parseChromaTOF(tofFiles[1])
```

---

parseELU *Parser for ELU files*

Description

Reads ASCII ELU-format files from AMDIS (Automated Mass Spectral Deconvolution and Identification System)

Usage

```
parseELU(f, min.pc = 0.01, mz = seq(50, 550), rt.cut = 0.008, rtrange = NULL)
```

Arguments

f	ELU filename to read.
min.pc	minimum percent of maximum intensity.
mz	vector of mass-to-charge bins of raw data table.
rt.cut	the difference in retention time, below which peaks are merged together.
rtrange	retention time range to parse peaks from, can speed up parsing if only interested in a small region (must be numeric vector of length 2)

Details

parseELU will typically be called by addAMDISPeaks, not called directly.

Peaks that are detected within rt.cut are merged together. This avoids peaks which are essentially overlapping.

Fragments that are less than min.pc of the maximum intensity fragment are discarded.

Value

list with components peaks (table of spectra – rows are mass-to-charge and columns are the different detected peaks) and tab (table of features for each detection), according to what is stored in the ELU file.

Author(s)

Mark Robinson

References

Mark D Robinson (2008). Methods for the analysis of gas chromatography - mass spectrometry data *PhD dissertation* University of Melbourne.

See Also

addAMDISPeaks

Examples

```
require(gcspikelite)

# paths and files
gcmsPath<-paste(find.package("gcspikelite"),"data",sep="/")
eluFiles<-dir(gcmsPath,"ELU",full=TRUE)

# parse ELU file
eluList<-parseELU(eluFiles[1])
```

---

peaksAlignment-class *Data Structure for pairwise alignment of 2 GCMS samples*

Description

Store the raw data and optionally, information regarding signal peaks for a number of GCMS runs

Usage

```
peaksAlignment(
  d1,
  d2,
  t1,
  t2,
  gap = 0.5,
  D = 50,
  timedf = NULL,
  df = 30,
  verbose = TRUE,
  usePeaks = TRUE,
  compress = TRUE,
  metric = 2,
  type = 2,
  penality = 0.2
)
```

Arguments

d1	matrix of MS intensities for 1st sample (if doing a peak alignment, this contains peak apexes/areas; if doing a profile alignment, this contains scan intensities. Rows are m/z bins, columns are peaks/scans.
d2	matrix of MS intensities for 2nd sample
t1	vector of retention times for 1st sample
t2	vector of retention times for 2nd sample
gap	gap penalty for dynamic programming algorithm. Not used if type=2
D	time window (on same scale as retention time differences, t1 and t2. Default scale is seconds.)
timedf	list (length = the number of pairwise alignments) of matrices giving the expected time differences expected at each pair of peaks used with usePeaks=TRUE.
df	integer, how far from the diagonal to go to calculate the similarity of peaks. Smaller value should run faster, but be careful not to choose too low.
verbose	logical, whether to print out info.
usePeaks	logical, TRUE uses peakdata list, FALSE uses rawdata list for computing similarity.
compress	logical, whether to compress the similarity matrix into a sparse format.
metric	numeric, different algorithm to calculate the similarity matrix between two mass spectrum. metric=1 call normDotProduct(); metric=2 call ndpRT(); metric=3 call corPrt()
type	numeric, two different type of alignment function
penality	penalization applied to the matching between two mass spectra if (t1-t2)>D

Details

peaksAlignment is a hold-all data structure of the raw and peak detection data.

Value

peaksAlignment object

Author(s)

Mark Robinson, Riccardo Romoli

References

Mark D Robinson (2008). Methods for the analysis of gas chromatography - mass spectrometry data *PhD dissertation* University of Melbourne.

See Also

peaksDataset, clusterAlignment

Examples

```
## see clusterAlignment, it calls peaksAlignment

## Not Run:
files <- list.files(path = paste(find.package("gcspikelite"), "data",
                    sep = "/"),"CDF", full = TRUE)
data <- peaksDataset(files[1:2], mz = seq(50, 550), rtrange = c(7.5, 8.5))
## create settings object
mfp <- xcms::MatchedFilterParam(fwhm = 10, snthresh = 5)
cwt <- xcms::CentWaveParam(snthresh = 3, ppm = 3000, peakwidth = c(3, 40),
 prefilter = c(3, 100), fitgauss = FALSE, integrate = 2, noise = 0,
 extendLengthMSW = TRUE, mzCenterFun = "wMean")
data <- addXCMSPeaks(files[1:2], data, settings = mfp)
data
plotChrom(data, rtrange=c(7.5, 10.5), runs=c(1:2))

## align two chromatogram
pA <- peaksAlignment(data@peaksdata[[1]], data@peaksdata[[2]],
                     data@peaksrt[[1]], data@peaksrt[[2]], D = 50,
                     metric = 3, compress = FALSE, type = 2, penality = 0.2)

plotAlignment(pA)
pA@v$match

par(mfrow=c(2,1))
plot(data@peaksdata[[1]][,15], type = 'h', main = paste(data@peaksrt[[1]][[15]]))
plot(data@peaksdata[[2]][,17], type = 'h',
     main = paste(data@peaksrt[[2]][[17]]))
## End (Not Run)
```

peaksDataset *Data Structure for raw GCMS data and peak detection results*

Description

Store the raw data and optionally, information regarding signal peaks for a number of GCMS runs

Usage

```
peaksDataset(
  fns = dir(, "[Cc][Dd][Ff]"),
  verbose = TRUE,
  mz = seq(50, 550),
  rtDivide = 60,
  rtrange = NULL
)
```

Arguments

fns	character vector, filenames of raw data in CDF format.
verbose	logical, if TRUE then iteration progress information is output.
mz	vector giving bins of raw data table.
rtDivide	number giving the amount to divide the retention times by.
rtrange	retention time range to limit data to (must be numeric vector of length 2)

Details

peaksDataset is a hold-all data structure of the raw and peak detection data.

Value

peaksDataset object

Author(s)

Mark Robinson

References

Mark D Robinson (2008). Methods for the analysis of gas chromatography - mass spectrometry data *PhD dissertation* University of Melbourne.

Examples

```
require(gcspikelite)

# paths and files
gcmsPath<-paste(find.package("gcspikelite"),"data",sep="/")
cdfFiles<-dir(gcmsPath,"CDF",full=TRUE)
eluFiles<-dir(gcmsPath,"ELU",full=TRUE)

# read data
pd<-peaksDataset(cdfFiles[1:2],mz=seq(50,550),rtrange=c(7.5,8.5))
show(pd)
```

---

plotAlignedFrags *plotAlignedFrags*

Description

Plot the aligned mass spectra

Usage

```
plotAlignedFrags(
  object,
  outList,
  specID,
  fullRange = TRUE,
  normalize = TRUE,
  ...
)
```

Arguments

object	where to keep the mass range of the experiment
outList	where to keep the mass spectra; both abundance than m/z
specID	a vector containing the index of the spectra to be plotted. Is referred to outList
fullRange	if TRUE uses the mass range of the whole experiment, otherwise uses only the mass range of each plotted spectum
normalize	if TRUE normalize the intensity of the mass peak to 100, the most abundant is 100% and the other peaks are scaled consequetially
...	further arguments passed to the 'plot' command

Details

Plot the deconvoluted and aligned mass spectra collected using gatherInfo()

Author(s)

Riccardo Romoli (riccardo.romoli@unifi.it)

Examples

```
files <- list.files(path = paste(find.package("gcspikelite"), "data",
                    sep = "/"),"CDF", full = TRUE)
data <- peaksDataset(files[1:4], mz = seq(50, 550), rtrange = c(7.5, 8.5))
## create settings object
mfp <- xcms::MatchedFilterParam(fwhm = 10, snthresh = 5)
cwt <- xcms::CentWaveParam(snthresh = 3, ppm = 3000, peakwidth = c(3, 40),
 prefilter = c(3, 100), fitgauss = FALSE, integrate = 2, noise = 0,
 extendLengthMSW = TRUE, mzCenterFun = "wMean")
data <- addXCMSPeaks(files[1:4], data, settings = mfp)
data
## multiple alignment
ma <- multipleAlignment(data, c(1,1,2,2), wn.gap = 0.5, wn.D = 0.05,
 bw.gap = 0.6, bw.D = 0.2, usePeaks = TRUE, filterMin = 1, df = 50,
 verbose = TRUE, metric = 2, type = 2)

## gather apex intensities
gip <- gatherInfo(data, ma)
gip[[33]]
plotAlignedFrags(object = data, outList = gip, specID = 33)
```

---

plotAlignment,peaksAlignment-method
plotAlignment

Description

Plotting functions for GCMS data objects

Usage

```
## S4 method for signature 'peaksAlignment'
plotAlignment(
  object,
  xlab = "Peaks - run 1",
  ylab = "Peaks - run 2",
  plotMatches = TRUE,
  matchPch = 19,
  matchLwd = 3,
  matchCex = 0.5,
  matchCol = "black",
  col = colorpanel(50, "white", "green", "navyblue"),
  breaks = seq(0, 1, length = 51),
  ...
)
```

Arguments

object	a clusterAlignment object
xlab	x-axis label
ylab	y-axis label
plotMatches	logical, whether to plot matches
matchPch	match plotting character
matchLwd	match line width
matchCex	match character expansion factor
matchCol	match colour
col	vector of colours for colourscale
breaks	vector of breaks for colourscale
...	further arguments passed to image

Details

Plot an object of peaksAlignment

The similarity matrix is plotted and optionally, the set of matching peaks. clusterAlignment objects are just a collection of all pairwise peakAlignment objects.

Value

plot an object of class peaksAlignment

Author(s)

Mark Robinson

References

Mark D Robinson (2008). Methods for the analysis of gas chromatography - mass spectrometry data *PhD dissertation* University of Melbourne.

See Also

peaksAlignment plotAlignment

Examples

```
require(gcspikelite)
files <- list.files(path = paste(find.package("gcspikelite"), "data",
                    sep = "/"),"CDF", full = TRUE)
data <- peaksDataset(files[1:2], mz = seq(50, 550), rtrange = c(7.5, 8.5))
## create settings object
mfp <- xcms::MatchedFilterParam(fwhm = 10, snthresh = 5)
cwt <- xcms::CentWaveParam(snthresh = 3, ppm = 3000, peakwidth = c(3, 40),
 prefilter = c(3, 100), fitgauss = FALSE, integrate = 2, noise = 0,
 extendLengthMSW = TRUE, mzCenterFun = "wMean")
```

```
data <- addXCMSPeaks(files[1:2], data, settings = mfp)
data
## image plot
plotChrom(data, rtrange = c(7.5,8.5), plotPeaks = TRUE, plotPeakLabels =TRUE)

## align two chromatogram
pA <- peaksAlignment(data@peaksdata[[1]], data@peaksdata[[2]],
                     data@peaksrt[[1]], data@peaksrt[[2]], D = 50,
                     compress = FALSE, type = 1, metric = 1,
                     gap = 0.5)
plotAlignment(pA)
```

---

plotChrom,peaksDataset-method

Plotting functions for GCMS data objects

Description

Store the raw data and optionally, information regarding signal peaks for a number of GCMS runs

Usage

```
## S4 method for signature 'peaksDataset'
plotChrom(
  object,
  runs = 1:length(object@rawdata),
  mzind = 1:nrow(object@rawdata[[1]]),
  mind = NULL,
  plotSampleLabels = TRUE,
  calcGlobalMax = FALSE,
  peakCex = 0.8,
  plotPeaks = TRUE,
  plotPeakBoundaries = FALSE,
  plotPeakLabels = FALSE,
  plotMergedPeakLabels = TRUE,
  mlwd = 3,
  usePeaks = TRUE,
  plotAcrossRuns = FALSE,
  overlap = F,
  rtrange = NULL,
  cols = NULL,
  thin = 1,
  max.near = median(object@rawrt[[1]]),
  how.near = 50,
  scale.up = 1,
  ...
)
```

Arguments

object	a peaksDataset object.
runs	set of run indices to plot
mzind	set of mass-to-charge indices to sum over (default, all)
mind	matrix of aligned indices
plotSampleLabels	logical, whether to display sample labels
calcGlobalMax	logical, whether to calculate an overall maximum for scaling
peakCex	character expansion factor for peak labels
plotPeaks	logical, whether to plot hashes for each peak
plotPeakBoundaries	logical, whether to display peak boundaries
plotPeakLabels	logical, whether to display peak labels
plotMergedPeakLabels	logical, whether to display 'merged' peak labels
mlwd	line width of lines indicating the alignment
usePeaks	logical, whether to plot alignment of peaks (otherwise, scans)
plotAcrossRuns	logical, whether to plot across peaks when unmatched peak is given
overlap	logical, whether to plot TIC/XICs overlapping
rtrange	vector of length 2 giving start and end of the X-axis
cols	vector of colours (same length as the length of runs)
thin	when usePeaks=FALSE, plot the alignment lines every thin values
max.near	where to look for maximum
how.near	how far away from max.near to look
scale.up	a constant factor to scale the TICs
...	further arguments passed to the plot

Details

Each TIC is scale to the maximum value (as specified by the how.near and max.near values). The many parameters gives considerable flexibility of how the TICs can be visualized.

Value

plot the chromatograms

Author(s)

Mark Robinson

References

Mark D Robinson (2008). Methods for the analysis of gas chromatography - mass spectrometry data *PhD dissertation* University of Melbourne.

See Also

peaksDataset

Examples

```
require(gcspikelite)

## paths and files
gcmsPath <- paste(find.package("gcspikelite"), "data", sep="/")
cdfFiles <- dir(gcmsPath, "CDF", full=TRUE)
eluFiles <- dir(gcmsPath, "ELU", full=TRUE)

## read data
pd <- peaksDataset(cdfFiles[1:3], mz=seq(50,550), rtrange=c(7.5,8.5))

## image plot
plotChrom(pd, rtrange = c(7.5,8.5), plotPeaks = TRUE,
          plotPeakLabels = TRUE)
```

---

plotClustAlignment,clusterAlignment-method
plotClustAlignment

Description

Plotting functions for GCMS data objects

Usage

```
## S4 method for signature 'clusterAlignment'
plotClustAlignment(object, alignment = 1, ...)
```

Arguments

object	clusterAlignment object.
alignment	the set of alignments to plot
...	further arguments passed to image. See also plotAlignment

Details

For clusterAlignment objects, the similarity matrix is plotted and optionally, the set of matching peaks. clusterAlignment objects are just a collection of all pairwise peakAlignment objects.

Value

plot the pairwise alignment

Author(s)

Mark Robinson

References

Mark D Robinson (2008). Methods for the analysis of gas chromatography - mass spectrometry data *PhD dissertation* University of Melbourne.

See Also

plotAlignment

Examples

```
require(gcspikelite)

# paths and files
gcmsPath <- paste(find.package("gcspikelite"), "data", sep="/")
cdfFiles <- dir(gcmsPath, "CDF", full=TRUE)
eluFiles <- dir(gcmsPath, "ELU", full=TRUE)

# read data, peak detection results
pd <- peaksDataset(cdfFiles[1:2], mz=seq(50,550), rtrange=c(7.5,8.5))
pd <- addAMDISPeaks(pd, eluFiles[1:2])

ca <- clusterAlignment(pd, gap=0.5, D=0.05, df=30, metric=1, type=1)
plotClustAlignment(ca, run = 1)
plotClustAlignment(ca, run = 2)
plotClustAlignment(ca, run = 3)
```

---

plotFrags *plotFrags*

Description

Plot the mass spectra from the profile matrix

Usage

```
plotFrags(object, sample, specID, normalize = TRUE, ...)
```

Arguments

object	an object of class "peaksDataset" where to keep the mass spectra; both abundance (y) than m/z (x)
sample	character, the sample from were to plot the mass spectra
specID	numerical, a vector containing the index of the spectra to be plotted.

normalize	logical, if TRUE normalize the intensity of the mass peak to 100, the most abundant is 100 consequetially
...	other parameter passed to the plot() function

Details

Plot the deconvoluted mass spectra from the profile matrix

Author(s)

riccardo.romoli@unifi.it

Examples

```
files <- list.files(path = paste(find.package("gcspikelite"), "data",
                    sep = "/"),"CDF", full = TRUE)
data <- peaksDataset(files[1:2], mz = seq(50, 550), rtrange = c(7.5, 8.5))
## create settings object
mfp <- xcms::MatchedFilterParam(fwhm = 10, snthresh = 5)
cwt <- xcms::CentWaveParam(snthresh = 3, ppm = 3000, peakwidth = c(3, 40),
 prefilter = c(3, 100), fitgauss = FALSE, integrate = 2, noise = 0,
 extendLengthMSW = TRUE, mzCenterFun = "wMean")
data <- addXCMSPeaks(files[1:2], data, settings = mfp)
data
## align two chromatogram
pA <- peaksAlignment(data@peaksdata[[1]], data@peaksdata[[2]],
                     data@peaksrt[[1]], data@peaksrt[[2]], D = 50,
                     metric = 3, compress = FALSE, type = 2, penality = 0.2)
pA@v$match
## plot the mass spectra
par(mfrow=c(2,1))
plotFrags(object=data, sample=1, specID=10)
plotFrags(object=data, sample=2, specID=12)
```

---

plotImage *Plot of images of GCMS data*

Description

Image plots (i.e. 2D heatmaps) of raw GCMS profile data

Usage

```
## S4 method for signature 'peaksDataset'
plotImage(
  object,
  run = 1,
  rtrange = c(11, 13),
```

```
  main = NULL,
  mzrange = c(50, 200),
  SCALE = log2,
  ...
)
```

Arguments

object	a peaksDataset object
run	index of the run to plot an image for
rtrange	vector of length 2 giving start and end of the X-axis (retention time)
main	main title (auto-constructed if not specified)
mzrange	vector of length 2 giving start and end of the Y-axis (mass-to-charge ratio)
SCALE	function called to scale the data (default: log2)
...	further arguments passed to the image command

Details

For peakDataset objects, each TIC is scale to the maximum value (as specified by the how.near and max.near values). The many parameters gives considerable flexibility of how the TICs can be visualized.

For peakAlignment objects, the similarity matrix is plotted and optionally, the set of matching peaks. clusterAlignment objects are just a collection of all pairwise peakAlignment objects.

Author(s)

Mark Robinson

References

Mark D Robinson (2008). Methods for the analysis of gas chromatography - mass spectrometry data *PhD dissertation* University of Melbourne.

See Also

plot, peaksDataset

Examples

```
require(gcspikelite)

# paths and files
gcmsPath<-paste(find.package("gcspikelite"),"data",sep="/")
cdfFiles<-dir(gcmsPath,"CDF",full=TRUE)
eluFiles<-dir(gcmsPath,"ELU",full=TRUE)

# read data
pd<-peaksDataset(cdfFiles[1],mz=seq(50,550),rtrange=c(7.5,8.5))
```

```
# image plot
plotImage(pd,run=1,rtrange=c(7.5,8.5),main="")
```

`progressiveAlignment-class`
Data Structure for progressive alignment of many GCMS samples

---

Description

Performs a progressive peak alignment (clustalw style) of multiple GCMS peak lists

Usage

```
progressiveAlignment(
  pD,
  cA,
  D = 50,
  gap = 0.5,
  verbose = TRUE,
  usePeaks = TRUE,
  df = 30,
  compress = FALSE,
  type = 2
)
```

Arguments

`pD`	a `peaksDataset` object
`cA`	a `clusterAlignment` object
`D`	retention time penalty
`gap`	gap parameter
`verbose`	logical, whether to print information
`usePeaks`	logical, whether to use peaks (if `TRUE`) or the full 2D profile alignment (if `FALSE`)
`df`	distance from diagonal to calculate similarity
`compress`	logical, whether to store the similarity matrices in sparse form
`type`	numeric, two different type of alignment function

Details

The progressive peak alignment we implemented here for multiple GCMS peak lists is analogous to how `clustalw` takes a set of pairwise sequence alignments and progressively builds a multiple alignment. More details can be found in the reference below.

Value

progressiveAlignment object

Author(s)

Mark Robinson

References

Mark D Robinson (2008). Methods for the analysis of gas chromatography - mass spectrometry data *PhD dissertation* University of Melbourne.

See Also

peaksDataset, multipleAlignment

Examples

```
require(gcspikelite)
files <- list.files(path = paste(find.package("gcspikelite"), "data",
                    sep = "/"),"CDF", full = TRUE)
data <- peaksDataset(files[1:2], mz = seq(50, 550), rtrange = c(7.5, 8.5))
## create settings object
mfp <- xcms::MatchedFilterParam(fwhm = 10, snthresh = 5)
cwt <- xcms::CentWaveParam(snthresh = 3, ppm = 3000, peakwidth = c(3, 40),
 prefilter = c(3, 100), fitgauss = FALSE, integrate = 2, noise = 0,
 extendLengthMSW = TRUE, mzCenterFun = "wMean")
data <- addXCMSPeaks(files[1:2], data, settings = mfp)
data
ca <- clusterAlignment(data, gap = 0.5, D = 0.05, df = 30, metric = 1,
  type = 1, compress = FALSE)
pa <- progressiveAlignment(data, ca, gap = 0.6, D = 0.1, df = 30,
 type = 1, compress = FALSE)
```

---

retFatMatrix *retFatMatrix*

Description

Build a fat data matrix

Usage

```
retFatMatrix(object, data, minFilter = round(length(object@files)/3 * 2))
```

Arguments

object	peakDataset object
data	a gatherInfo() object
minFilter	the minimum number for a feature to be returned in the data matrix. Default is 2/3 of the samples

Details

This function allows to extract the data from an object created using gatherInfo and build a data matrix using the area of the deconvoluted and aligned peaks. The row are the samples while the column represent the different peaks.

Value

A fat data matrix containing the area of the deconvoluted and aligned peaks. The row are the samples while the column represent the different peaks

Author(s)

Riccardo Romoli <riccardo.romoli@unifi.it>

See Also

gatherInfo

Examples

```
require(gcspikelite)
files <- list.files(path = paste(find.package("gcspikelite"), "data",
                    sep = "/"),"CDF", full = TRUE)
data <- peaksDataset(files[1:2], mz = seq(50, 550), rtrange = c(7.5, 8.5))
## create settings object
mfp <- xcms::MatchedFilterParam(fwhm = 10, snthresh = 5)
cwt <- xcms::CentWaveParam(snthresh = 3, ppm = 3000, peakwidth = c(3, 40),
 prefilter = c(3, 100), fitgauss = FALSE, integrate = 2, noise = 0,
 extendLengthMSW = TRUE, mzCenterFun = "wMean")
data <- addXCMSPeaks(files[1:2], data, settings = mfp)
data
ma <- multipleAlignment(pd = data, group = c(1,1),
                        filterMin = 1, metric = 2, type = 2)
outList <- gatherInfo(data, ma)
mtxD <- retFatMatrix(object = data, data = outList, minFilter = 1)
```

rmaFitUnit *Fits a robust linear model (RLM) for one metabolite*

Description

Using rlm from MASS, this procedure fits a linear model using all the fragments

Usage

```
rmaFitUnit(
  u,
  maxit = 5,
  mzEffect = TRUE,
  cls = NULL,
  fitSample = TRUE,
  fitOrCoef = c("coef", "fit"),
  TRANSFORM = log2
)
```

Arguments

u	a metabolite unit (list object with vectors mz and rt for m/z and retention times, respectively and a data element giving the fragmentxsample intensitity matrix)
maxit	maximum number of iterations (default: 5)
mzEffect	logical, whether to fit m/z effect (default: TRUE)
cls	class variable
fitSample	whether to fit individual samples (alternative is fit by group)
fitOrCoef	whether to return a vector of coefficients (default: "coef"), or an rlm object ("fit")
TRANSFORM	function to transform the raw data to before fitting (default: log2)

Details

Fits a robust linear model.

Value

list giving elements of fragment and sample coefficients (if fitOrCoef="coef") or a list of elements from the fitting process (if fitOrCoef="fit")

Author(s)

Mark Robinson

References

Mark D Robinson (2008). Methods for the analysis of gas chromatography - mass spectrometry data *PhD dissertation* University of Melbourne.

See Also

peaksAlignment, clusterAlignment

Examples

```
require(gcspikelite)

# paths and files
gcmsPath<-paste(find.package("gcspikelite"),"data",sep="/")
cdfFiles<-dir(gcmsPath,"CDF",full=TRUE)
eluFiles<-dir(gcmsPath,"ELU",full=TRUE)

# read data, peak detection results
pd<-peaksDataset(cdfFiles[1:2],mz=seq(50,550),rtrange=c(7.5,8.5))
pd<-addAMDISPeaks(pd,eluFiles[1:2])

# pairwise alignment using all scans
fullca<-clusterAlignment(pd, usePeaks = FALSE, df = 100)

# calculate retention time shifts
timedf<-calcTimeDiffs(pd, fullca)
```

---

show,multipleAlignment-method

Store the raw data and optionally, information regarding signal peaks for a number of GCMS runs

---

Description

multipleAlignment is the data structure giving the result of an alignment across several GCMS runs. Multiple alignments are done progressively. First, all samples with the same `tg$Group` label with be aligned (denoted a "within" alignment). Second, each group will be summarized into a pseudo-data set, essentially a spectrum and retention time for each matched peak of the within-alignment. Third, these "merged peaks" are aligned in the same progressive manner, here called a "between" alignment.

Usage

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

Arguments

`object`	multipleAlignment object

Author(s)

Mark Robinson

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