Package 'CluMSID'

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Type Package

Title Clustering of MS2 Spectra for Metabolite Identification

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Description CluMSID is a tool that aids the identification of features in untargeted LC-MS/MS analysis by the use of MS2 spectra similarity and unsupervised statistical methods. It offers functions for a complete and customisable workflow from raw data to visualisations and is interfaceable with the xmcs family of preprocessing packages.

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BugReports https://github.com/tdepke/CluMSID/issues

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Contents

`accessors` *Accessor functions for individual slots of* `MS2spectrum` *and* `pseudospectrum` *objects*

Description

Accessor functions for individual slots of `MS2spectrum` and `pseudospectrum` objects

Usage

```
accessID(x)

accessAnnotation(x)

accessPrecursor(x)

accessRT(x)

accessPolarity(x)
```

```
accessSpectrum(x)

accessNeutralLosses(x)
```

Arguments

x	An object of class MS2spectrum or pseudospectrum

Value

The value of the respective slot of the object (id, annotation, precursor, rt, spectrum, neutral_losses)

Examples

```
load(file = system.file("extdata",
    "annotatedSpeclist.RData",
    package = "CluMSIDdata"))

accessID(annotatedSpeclist[[1]])

load(file = system.file("extdata",
    "annotatedSpeclist.RData",
    package = "CluMSIDdata"))

accessAnnotation(annotatedSpeclist[[1]])

load(file = system.file("extdata",
    "annotatedSpeclist.RData",
    package = "CluMSIDdata"))

accessPrecursor(annotatedSpeclist[[1]])

load(file = system.file("extdata",
    "annotatedSpeclist.RData",
    package = "CluMSIDdata"))

accessRT(annotatedSpeclist[[1]])

load(file = system.file("extdata",
    "annotatedSpeclist.RData",
    package = "CluMSIDdata"))

accessPolarity(annotatedSpeclist[[1]])

load(file = system.file("extdata",
    "annotatedSpeclist.RData",
    package = "CluMSIDdata"))

accessSpectrum(annotatedSpeclist[[1]])

load(file = system.file("extdata",
    "annotatedSpeclist.RData",
    package = "CluMSIDdata"))

accessNeutralLosses(annotatedSpeclist[[1]])
```

addAnnotations *Adding external annotations to list of* MS2spectrum *objects*

Description

addAnnotations is used to add annotations that have been assigned externally, e.g. by library search, to a list of MS2spectrum objects as produced by extractMS2spectra and mergeSpecList.

Usage

```
addAnnotations(featlist, annolist, annotationColumn = 4)
```

Arguments

featlist	A list of MS2spectrum objects as produced by extractMS2spectra and mergeSpecList
annolist	A list of annotations, either as a data.frame or csv file. The order of features must be the same as in featlist. Please see the package vignette for a detailed example!
annotationColumn	The column of annolist were the annotation is found. Default is 4, which is the case if writeFeaturelist followed by manual addition of annotations, e.g. in Excel, is used to generate annolist.

Value

A list of MS2spectrum objects as produced by extractMS2spectra and mergeSpecList with external annotations added to the annotation slot of each MS2spectrum object.

Examples

```
load(file = system.file("extdata",
    "featlist.RData",
    package = "CluMSIDdata"))

addAnnotations(featlist, system.file("extdata",
                "post_anno.csv",
                package = "CluMSIDdata"),
                annotationColumn = 4)
```

as.MS2spectrum *Convert spectra from* **MSnbase** *classes*

Description

Convert spectra from **MSnbase** classes

Usage

```
as.MS2spectrum(x)
```

Arguments

x	An object of class Spectrum or Spectrum2

Value

An object of class MS2spectrum

Examples

```
#Load a "Spectrum2" object from MSnbase
library(MSnbase)
sp <- itraqdata[["X1"]]
#Convert this object to "MS2spectrum" class
new_sp <- as.MS2spectrum(sp)
#Or alternatively:
new_sp <- as(sp, "MS2spectrum")
```

---

cossim *Calculate cosine similarity between two spectra*

Description

cossim() calculates the cosine of the spectral constrast angle as a measure for the similarity of two spectra.

Usage

```
cossim(x, y, type = c("spectrum", "neutral_losses"),
    mzTolerance = 1e-05)

## S4 method for signature 'MS2spectrum,MS2spectrum'
cossim(x, y, type = c("spectrum",
    "neutral_losses"), mzTolerance = 1e-05)

## S4 method for signature 'pseudospectrum,pseudospectrum'
cossim(x, y,
    type = c("spectrum", "neutral_losses"), mzTolerance = 1e-05)
```

Arguments

x, y	MS2 spectra, either as matrix, MS2spectrum or pseudospectrum objects. x and y must have the same class.
type	Whether similarity between spectra ("spectrum", default) or neutral loss patterns ("neutral_losses") is to be compared
mzTolerance	The m/z tolerance used for merging. If two fragment peaks are within tolerance, they are regarded as the same. Defaults to 1e-5, i.e. 10ppm.

Value

The cosine similarity of x and y

Methods (by class)

- x = MS2spectrum, y = MS2spectrum: cossim method for MS2spectrum objects
- x = pseudospectrum, y = pseudospectrum: cossim method for pseudospectrum objects

Examples

```
load(file = system.file("extdata",
    "annotatedSpeclist.RData",
    package = "CluMSIDdata"))

cossim(annotatedSpeclist[[1]], annotatedSpeclist[[2]])
```

---

distanceMatrix *Create distance matrix from list of spectra*

Description

distanceMatrix() creates a distance matrix from a list of MS2 spectra, MS1 pseudospectra or neutral loss patterns by pairwise comparison using the specified distance function. This distance matrix is the basis for CluMSID's data mining functions.

Usage

```
distanceMatrix(speclist, distFun = "cossim", type = c("spectrum",
    "neutral_losses"), mz_tolerance = 1e-05)
```

Arguments

speclist	A list of MS2spectrum or pseudospectrum objects as generated by extractMS2spectra or extractPseudospectra.
distFun	The distance function to be used. At the moment, only cossim is implemented.
type	"spectrum" (default) for MS2 spectra or MS1 pseudospectra or "neutral_losses" for neutral loss patterns.
mz_tolerance	The *m/z* tolerance to be used for merging, default is 1e-5, i.e. +/- 10ppm. If the mass-to-charge ratios of two peaks differ less than *mz_tolerance*, they are assumed to have the same *m/z*

Value

A numeric length(speclist) by length(speclist) matrix containing pairwise distances (1 - similarity) between all features in speclist. Row and column names are taken from the id slot or, if present, pasted from the id and annotation slots of the MS2spectrum or pseudospectrum objects.

Examples

```
load(file = system.file("extdata",
    "annotatedSpeclist.RData",
    package = "CluMSIDdata"))

distanceMatrix(annotatedSpeclist[1:20])
```

extractMS2spectra *Extract MS2 spectra from raw data files*

Description

`extractMS2spectra()` is used to extract MS2 spectra from raw data files, e.g. mzXML files.

Usage

```
extractMS2spectra(MSfile, min_peaks = 2, recalibrate_precursor = FALSE,
    RTlims = NULL)
```

Arguments

`MSfile`	An LC-MS/MS raw data file in one of the non-proprietary formats that can be parsed by `mzR`, e.g. mzXML or mzML.
`min_peaks`	Minimum number of peaks in MS2 spectrum, defaults to `2`. Spectra with less than `min_peaks` fragment peaks will be ignored and not extracted.
`recalibrate_precursor`	Logical, defaults to `FALSE`. Applicable only for files that were exported to mzXML using a deprecated version of Bruker Compass Xport (< 3.0.13). If set to `TRUE`, the precursor m/z will be recalculated from the respective fragment m/z in the MS2 spectrum. For details, see Depke et al. 2017.
`RTlims`	Retention time interval for the extraction of spectra. Provide as numeric vector of length 2. Spectra with retention time < `RTlims[1]` or > `RTlims[2]` will be ignored.

Value

A `list` with objects of class `MS2spectrum`, containing MS2 spectra extracted from the raw data.

Examples

```
my_spectra <- extractMS2spectra(MSfile = system.file("extdata",
                                "PoolA_R_SE.mzXML",
                                package = "CluMSIDdata"),
                                min_peaks = 4, RTlims = c(0,10))
```

extractPseudospectra *Extract pseudospectra*

Description

`extractPseudospectra()` is used to extract MS1 pseudospectra from **CAMERA** output.

Usage

```
extractPseudospectra(x, min_peaks = 1, intensity_columns = NULL)
```

Arguments

x	**CAMERA** output that contains information on pseudospectra. Can either be of class data.frame or xsAnnotate. It is recommended to use either xsAnnotate objects or data.frames generated from XCMSonline results tables but other data.frames are possible.
min_peaks	Minimum number of peaks in pseudospectrum, defaults to 1. See extractMS2spectra.
intensity_columns	Numeric, defaults to NULL. If a data.frame is used as input which has not been generated from an XCMSonline results table, the indices of the columns that contain the peak intensities in the different samples have to be indicated as intensity_columns.

Value

A list of pseudospectra, stored as objects of class pseudospectrum, analogous to the output of extractMS2spectra.

Examples

```
pstable <- readr::read_delim(file = system.file("extdata",
                                "TD035_XCMS.annotated.diffreport.tsv",
                                package = "CluMSIDdata"), delim = "\t")

pseudospeclist <- extractPseudospectra(pstable, min_peaks = 2)
```

---

featureList *Generate a* data.frame *with feature information from list of* MS2spectrum *objects*

Description

featureList generates a data.frame that contains feature ID, precurosur *m/z* and retention time for all features contained in a list of MS2spectrum objects as produced by extractMS2spectra and mergeSpecList. featureList is used internally by writeFeaturelist.

Usage

```
featureList(featlist)
```

Arguments

featlist	A list of MS2spectrum objects as produced by extractMS2spectra and mergeSpecList

Details

Although originally designed for lists of MS2spectrum objects, the function also works with lists of pseudospectrum objects. In this case, NA is given for precursor *m/z*.

Value

A data.frame that contains feature ID, precurosur *m/z* (if available) and retention time

Examples

```
load(file = system.file("extdata",
    "featlist.RData",
    package = "CluMSIDdata"))

pre_anno <- featureList(featlist)
```

`findFragment` *Find spectra that contain a specific fragment*

Description

`findFragment` is used to find spectra that contain a specific fragment ion. Its sister function is `findNL`, which finds specific neutral losses. Both functions work analogous to `getSpectrum`.

Usage

```
findFragment(featlist, mz, tolerance = 1e-05)
```

Arguments

`featlist`	a list that contains only objects of class `MS2spectrum`
`mz`	The mass-to-charge ratio of the fragment ion of interest.
`tolerance`	The *m/z* tolerance for the fragment ion search. Default is `1E-05`, i.e. +/- 10ppm.

Value

If the respective fragment is only found in one spectrum, the output is an object of class `MS2spectrum`; if it is found in more than one spectrum, the output is a list of `MS2spectrum` objects.

Examples

```
load(file = system.file("extdata",
    "annotatedSpeclist.RData",
    package = "CluMSIDdata"))
putativeAQs <- findFragment(annotatedSpeclist, 159.068)
```

`findNL` *Find spectra that contain a specific neutral loss*

Description

`findNL` is used to find spectra that contain a specific neutral loss. Its sister function is `findFragment`, which finds specific fragment ions. Both functions work analogous to `getSpectrum`.

Usage

```
findNL(featlist, mz, tolerance = 1e-05)
```

Arguments

featlist	a list that contains only objects of class MS2spectrum
mz	The mass-to-charge ratio of the neutral loss of interest.
tolerance	The *m/z* tolerance for the neutral loss search. Default is 1E-05, i.e. +/- 10ppm.

Value

If the respective neutral loss is only found in one spectrum, the output is an object of class MS2spectrum; if it is found in more than one spectrum, the output is a list of MS2spectrum objects.

Examples

```
load(file = system.file("extdata",
    "annotatedSpeclist.RData",
    package = "CluMSIDdata"))
findNL(annotatedSpeclist, 212.009)
```

---

getSimilarities *Match one spectrum against a set of spectra*

Description

getSimilarities calculates the similarities of one spectrum or neutral loss pattern to a set of other spectra or neutral loss patterns.

Usage

```
getSimilarities(spec, speclist, type = c("spectrum", "neutral_losses"),
    hits_only = FALSE)
```

Arguments

spec	The spectrum to be compared to other spectra. Can be either an object of class MS2spectrum or a two-column numerical matrix that contains fragment mass-to-charge ratios in the first and intensities in the second column.
speclist	The set of spectra to which spec is to be compared. Must be a list where every entry is an object of class MS2spectrum. Can be generated from an mzXML file with extractMS2spectra and mergeMS2spectra or constructed using new("MS2spectrum", ...) for every list entry (see vignette for details).
type	Specifies whether MS2 spectra or neutral loss patterns are to be compared. Must be either 'spectrum' (default) or 'neutral_losses'.
hits_only	Logical that indicates whether the result should contain only similarities greater than zero.

Value

A named vector with similarities of spec to all spectra or neutral loss patterns in speclist.

Examples

```
load(file = system.file("extdata",
    "annotatedSpeclist.RData",
    package = "CluMSIDdata"))
getSimilarities(annotatedSpeclist[[137]],
                annotatedSpeclist, hits_only = TRUE)
```

`getSpectrum` *Access individual spectra from a list of spectra by various slot entries*

Description

As accessing S4 objects within lists is not trivial, `getSpectrum` can be used to access individual or several `MS2spectrum` objects by their slot entries.

Usage

```
getSpectrum(featlist, slot, what, mz.tol = 1e-05, rt.tol = 30)
```

Arguments

`featlist`	a list that contains only objects of class `MS2spectrum`
`slot`	The slot to be searched (invalid slot arguments will produce errors). Possible values are: • `'id'` • `'annotation'` • `'precursor'` (*m/z* of precursor ion) • `'rt'` (retention time of precursor)
`what`	the search term or number, must be character for `'id'` and `'annotation'` and numeric for `'precursor'` and `'rt'` See vignette for examples.
`mz.tol`	the tolerance used for precursor ion *m/z* searches, defaults to `1E-05` (+/- 10ppm)
`rt.tol`	the tolerance used for precursor ion retention time searches, defaults to 30s; high values can be used to specify retention time ranges (see vignette for example)

Value

If the only one spectrum matches the search criteria, the output is an object of class `MS2spectrum`; if more than one spectrum matches, the output is a list of `MS2spectrum` objects.

Examples

```
load(file = system.file("extdata",
    "annotatedSpeclist.RData",
    package = "CluMSIDdata"))

getSpectrum(annotatedSpeclist, "annotation", "pyocyanin")

getSpectrum(annotatedSpeclist, "id", "M244.17T796.4")
```

```
getSpectrum(annotatedSpeclist, "precursor", 286.18, mz.tol = 1E-03)

six_eight <- getSpectrum(annotatedSpeclist, "rt", 420, rt.tol = 60)
```

HCplot *Generate cluster dendrogram or heatmap from spectral similarity data*

Description

`HCplot()` performs hierarchical clustering of spectral similarity data using average linkage as agglomeration criterion like `HCtbl` and generates either a circular dendrogram or a combination of dendrogram and heatmap.

Usage

```
HCplot(distmat, h = 0.95, type = c("dendrogram", "heatmap"), ...)
```

Arguments

`distmat`	A distance matrix as generated by `distanceMatrix`.
`h`	Height where the tree is to be cut, defaults to `0.95`. See `cutree` for details.
`type`	Specifies which visualisation is to be generated: `"dendrogram"` (default) for a circular dendrogram or `"heatmap"` for a combination of dendrogram and heatmap.
`...`	Additional graphical parameters passed to `plot.phylo` (for `type = "dendrogram"`) or `gplots::heatmap.2` (for `type = "heatmap"`)

Value

A plot as specified by `type`.

Examples

```
load(file = system.file("extdata",
    "distmat.RData",
    package = "CluMSIDdata"))

HCplot(distmat[1:50,1:50], h = 0.8, type = "heatmap")
```

HCtbl *Hierarchical clustering of spectral similarity data*

Description

HCtbl() performs hierarchical clustering of spectral similarity data using average linkage as agglomeration criterion.

Usage

```
HCtbl(distmat, h = 0.95)
```

Arguments

distmat	A distance matrix as generated by distanceMatrix.
h	Height where the tree is to be cut, defaults to 0.95. See cutree for details.

Value

A data.frame with name and cluster ID for each feature in distmat.

See Also

HCplot

Examples

```
load(file = system.file("extdata",
    "distmat.RData",
    package = "CluMSIDdata"))

my_HCtbl <- HCtbl(distmat[1:50,1:50], h = 0.8)
```

MDSplot *Multidimensional scaling of spectral similarity data*

Description

MDSplot() is used to generate multidimensional scaling plots from spectral similarity data. An interactive visualisation can be produced using **plotly**.

Usage

```
MDSplot(distmat, interactive = FALSE, highlight_annotated = FALSE, ...)
```

Arguments

distmat	A distance matrix as generated by distanceMatrix.
interactive	Logical, defaults to FALSE. If TRUE, an interactive visualisation is generated using **plotly**.
highlight_annotated	Logical, defaults to FALSE. If TRUE, points for features for which an annotation was added before using distanceMatrix are highlighted by red colour, while other points are grey in the MDS plot.
...	Additional arguments passed to geom_point(), e.g. pch, size or alpha.

Value

An MDS plot generated with the help of cmdscale, ggplot and, if interactive, ggplotly.

Examples

```
load(file = system.file("extdata",
    "distmat.RData",
    package = "CluMSIDdata"))

MDSplot(distmat, highlight_annotated = TRUE)
```

---

mergeMS2spectra *Merge MS2 spectra with or without external peak table*

Description

mergeMS2spectra is used to merge MS2 spectra that come from the same precursor. It does so either by grouping spectra of the same precursor *m/z* that fall into a defined retention time window (rt_tolerance) or by grouping spectra to peaks from an externally supplied peak table. Please see the vignette for more details.

Usage

```
mergeMS2spectra(ms2list, mz_tolerance = 1e-05, rt_tolerance = 30,
    peaktable = NULL, exclude_unmatched = FALSE)
```

Arguments

ms2list	A list of MS2spectrum objects to be merged.
mz_tolerance	The *m/z* tolerance to be used for merging, default is 1e-5, i.e. +/- 10ppm. If the mass-to-charge ratios of two peaks differ less than *mz_tolerance*, they are assumed to have the same *m/z*
rt_tolerance	The retention time tolerance used for merging features. If used without a peak table, rt_tolerance is the maximum retention time difference between to subsequent spectra of the same precursor *m/z* with which they are still assumed to belong to the same feature If used with an external peak table, rt_tolerance is the maximum retention time difference between a spectrum and a peak in the peak table with which the spectrum is still considered to belong to that peak.

peaktable — An external peak table, e.g. from XCMS, that serves as a template for grouping spectra. The peaktable must be a three-column `data.frame` with feature ID, *m/z* and retention time for each peak/feature.

exclude_unmatched — If an external peak table is used: Should spectra that do not match to any peak/feature in the peak table be exclude from the resulting list?

Value

A merged list of `MS2spectrum` objects.

Examples

```
my_spectra <- extractMS2spectra(MSfile = system.file("extdata",
                                "PoolA_R_SE.mzXML",
                                package = "CluMSIDdata"),
                                min_peaks = 4, RTlims = c(0,5))

my_merged_spectra <- mergeMS2spectra(my_spectra, rt_tolerance = 20)
```

---

mergeSpecList *Merge list of spectra*

Description

`mergeSpecList()` is an accessory function used only inside `mergeMS2spectra`.

Usage

```
mergeSpecList(speclist, tolerance = 1e-05)
```

Arguments

speclist — A `list` of `MS2spectrum` objects to be merged.

tolerance — The m/z tolerance to be used for merging.

Value

A `list` of the same length as `speclist` containing merged spectra as `MS2spectrum` objects. If multiple spectra contribute to one consensus spectrum, than this consensus spectrum is contained in the list multiple times at the respective positions of the contributing spectra.

`mergeTolerance` *Merge spectra with m/z tolerance*

Description

`mergeTolerance()` merges two spectra by identifying common peaks with a given m/z tolerance. It can be used with `Reduce()` to merge more than two spectra.

Usage

```
mergeTolerance(x, y, tolerance = 1e-05)
```

Arguments

`x, y`	MS2 spectra as objects of class `matrix` with m/z in the first column and intensity in the second.
`tolerance`	The m/z tolerance used for merging. If two peaks are within tolerance, they are regarded as the same. Defaults to `1e-5`, i.e. 10ppm.

Value

A matrix with m/z in the first column and separate columns for intensities in the respective spectra. If peaks were merged, their m/z corresponds to the mean of the two original m/z.

`MS2spectrum-class` *A custom S4 class for MS2 spectra, neutral loss patterns and respective metainformation*

Description

A custom S4 class for MS2 spectra, neutral loss patterns and respective metainformation

Usage

```
## S4 method for signature 'MS2spectrum'
show(object)

## S4 method for signature 'MS2spectrum'
precursorMz(object)

## S4 method for signature 'MS2spectrum'
rtime(object)

## S4 method for signature 'MS2spectrum'
intensity(object)

## S4 method for signature 'MS2spectrum'
mz(object)

## S4 method for signature 'MS2spectrum,ANY'
peaksCount(object)
```

Arguments

object	An object of class MS2spectrum

Value

Prints information from the object slots with exception of 'spectrum' and 'neutral_losses' where only a summary is given.

Methods (by generic)

- show: A show generic for MS2spectra.
- precursorMz: Method forMSnbase::precursorMz for MS2spectrum objects. Accesses precursor slot and returns precursor *m/z* as a numeric.
- rtime: Method forMSnbase::rtime for MS2spectrum objects. Accesses rt slot and returns retention time as a numeric.
- intensity: Method forMSnbase::intensity for MS2spectrum objects. Accesses spectrum slot and returns the intensity column as a numeric vector.
- mz: Method forMSnbase::mz for MS2spectrum objects. Accesses spectrum slot and returns the *m/z* column as a numeric vector.
- peaksCount: Method forMSnbase::mz for MS2spectrum objects. Accesses spectrum slot and returns the number of peaks as a numeric.

Slots

id a character string similar to the ID used by XCMSonline or the ID given in a predefined peak list

annotation a character string containing a user-defined annotation, defaults to empty

precursor (median) *m/z* of the spectrum's precursor ion

rt (median) retention time of the spectrum's precursor ion

polarity the ionisation polarity, "positive" or "negative"

spectrum the actual MS2 spectrum as two-column matrix (column 1 is (median) *m/z*, column 2 is (median) intensity of the product ions)

neutral_losses a neutral loss pattern generated by subtracting the product ion mass-to-charge ratios from the precursor *m/z* in a matrix format analogous to the spectrum slot

---

networkplot *Correlation network from spectral similarity data*

Description

networkplot() is used to generate correlation networks from spectral similarity data. An interactive visualisation can be produced using **plotly**.

Usage

```
networkplot(distmat, interactive = FALSE, show_labels = FALSE,
    label_size = 1.5, highlight_annotated = FALSE,
    min_similarity = 0.1, exclude_singletons = FALSE)
```

Arguments

distmat	A distance matrix as generated by distanceMatrix.
interactive	Logical, defaults to FALSE. If TRUE, an interactive visualisation is generated using **plotly**.
show_labels	Logical, defaults to FALSE. If TRUE, feature IDs are printed as labels in the network plot. Argument has no effect if interactive is TRUE (because in this case, labels are displayed on mouse-over).
label_size	Numeric, defaults to 1.5. If show_labels is TRUE and interactive is FALSE, label_size defines the size of labels in the plot.
highlight_annotated	Logical, defaults to FALSE. If TRUE, points for features for which an annotation was added before using distanceMatrix are highlighted by red colour, while other points are grey in the network plot.
min_similarity	Numeric, defaults to 0.1. The minimum spectral contrast angle (seecossim) that is considered a spectral similarity and hence a connection in the network.
exclude_singletons	Logical, defaults to FALSE. If TRUE, features that have no connection to any other feature will not be displayed in the network plot.

Value

A network plot generated with the help of network, ggnet2 and, if interactive, ggplotly. Edge weights correspond to spectral similarities.

Examples

```
load(file = system.file("extdata",
    "distmat.RData",
    package = "CluMSIDdata"))

networkplot(distmat[1:50,1:50], show_labels = TRUE,
                exclude_singletons = TRUE)
```

---

neutrallossPatterns *Generate neutral loss patterns from MS2 spectra*

Description

neutrallossPatterns generates neutral loss patterns from MS2 spectra and adds them to MS2spectrum objects in the slot neutral_losses.

Usage

```
neutrallossPatterns(x)
```

Arguments

x	an object of class MS2spectrum that contains an MS2 spectrum in the spectrum slot

Value

an object of class MS2spectrum with a neutral loss pattern in the neutral_losses slot

---

OPTICSplot *Visualisation of density-based clustering of spectral similarity data*

Description

OPTICSplot() performs density-based clustering of spectral similarity data using the OPTICS algorithm like OPTICStbl and creates a reachability distance plot.

Usage

```
OPTICSplot(distmat, eps = 10000, minPts = 3, eps_cl = 0.5, ...)
```

Arguments

distmat	A distance matrix as generated by distanceMatrix.
eps	OPTICS parameters, see optics.
minPts	OPTICS parameters, see optics.
eps_cl	The reachability distance used for cluster determination, see extractDBSCAN.
...	Additional graphical parameters to be passed to plot()

Details

The function internally uses optics and extractDBSCAN from the **dbscan** package.

Value

A reachability distance plot as visualisation of OPTICS clustering, see codeextractDBSCAN.

See Also

OPTICStbl

Examples

```
load(file = system.file("extdata",
    "distmat.RData",
    package = "CluMSIDdata"))

OPTICSplot(distmat[1:50,1:50], eps_cl = 0.7)
```

OPTICStbl *Density-based clustering of spectral similarity data*

Description

`OPTICStbl()` performs density-based clustering of spectral similarity data using the OPTICS algorithm.

Usage

```
OPTICStbl(distmat, eps = 10000, minPts = 3, eps_cl = 0.5)
```

Arguments

`distmat`	A distance matrix as generated by `distanceMatrix`.
`eps`, `minPts`	OPTICS parameters, see `optics`.
`eps_cl`	The reachability distance used for cluster determination, see `extractDBSCAN`.

Details

The function internally uses `optics` and `extractDBSCAN` from the **dbscan** package.

Value

A `data.frame` with feature name, cluster ID and OPTICS order for each feature in `distmat`.

See Also

OPTICSplot

Examples

```
load(file = system.file("extdata",
    "distmat.RData",
    package = "CluMSIDdata"))

my_OTPICStbl <- OPTICStbl(distmat[1:50,1:50], eps_cl = 0.7)
```

pseudospectrum-class *A custom S4 class for MS1 pseudospectra and respective metainformation*

Description

A custom S4 class for MS1 pseudospectra and respective metainformation

Slots

`id` a the "pcgroup" number assigned by **CAMERA**

`annotation` a character string containing a user-defined annotation, defaults to empty

`rt` (median) retention time of the ions contained in the pseudospectrum

`spectrum` the actual MS1 pseudospectrum as two-column matrix (column 1 is (median) *m/z*, column 2 is (median) intensity of the ions)

---

specplot *Create a basic plot of MS2 spectra*

Description

`specplot` creates a very basic plot of MS2 spectra from `MS2spectrum` or `pseudospectrum` objects.

Usage

```
specplot(spec, ...)
```

Arguments

`spec`	An object of class `MS2spectrum` or `pseudospectrum`
`...`	Additional graphical parameters to be passed to `plot()`

Value

A plot of the MS2 spectrum saved in the `spectrum` slot of `spec`.

Examples

```
load(file = system.file("extdata",
    "annotatedSpeclist.RData",
    package = "CluMSIDdata"))

specplot(annotatedSpeclist[[1]])
```

---

splitPolarities *Separate spectra with different polarities from the same run*

Description

Using `splitPolarities`, spectra with different polarities from the same run can be separated, e.g. when processing spectra recorded with polarity-switching.

Usage

```
splitPolarities(ms2list, polarity = c("positive", "negative"))
```

Arguments

ms2list	A list of MS2spectrum objects as produced by extractMS2spectra.
polarity	The polarity of spectra to be analysed, must be "positive" or "negative".

Value

A list of MS2spectrum objects that contains only spectra with the given polarity.

Examples

```
my_spectra <- extractMS2spectra(MSfile = system.file("extdata",
                                "PoolA_R_SE.mzXML",
                                package = "CluMSIDdata"),
                                min_peaks = 4, RTlims = c(0,5))

my_positive_spectra <- splitPolarities(my_spectra, "positive")
```

---

writeFeaturelist *Write feature information from list of* MS2spectrum *objects*

Description

writeFeaturelist uses featureList to generate a data.frame that contains feature ID, precurosur *m/z* and retention time for all features contained in a list of MS2spectrum objects as produced by extractMS2spectra and mergeSpecList and writes it to a csv file.

Usage

```
writeFeaturelist(featlist, filename = "pre_anno.csv")
```

Arguments

featlist	A list of MS2spectrum objects as produced by extractMS2spectra and mergeSpecList
filename	The desired file name of the csv file, default is "pre_anno.csv"

Details

Although originally designed for lists of MS2spectrum objects, the function also works with lists of pseudospectrum objects. In this case, NA is given for precursor *m/z*.

Value

A csv file that contains feature ID, precurosur *m/z* and retention time. The file has a header but no row names and is separated by ','.

Examples

```
load(file = system.file("extdata",
    "featlist.RData",
    package = "CluMSIDdata"))

writeFeaturelist(featlist, filename = "pre_anno.csv")
```

Index