

Package ‘MetCirc’

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Type Package

Title Navigating mass spectral similarity in high-resolution MS/MS metabolomics data

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Author Thomas Naake <thomasnaake@googlemail.com> and Emmanuel Gaquerel
<emmanuel.gaquerel@cos.uni-heidelberg.de>

Maintainer Thomas Naake <thomasnaake@googlemail.com>

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Description MetCirc comprises a workflow to interactively explore high-resolution MS/MS metabolomics data: create an MSP object, a format for MS/MS library data, bin m/z values of precursors, calculate similarity between precursors based on the normalised dot product and visualise similarities in a circular layout. Within the interactive framework the user can annotate MS/MS features based on their similarity to (known) related MS/MS features.

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adduct*adduct returns adduct ion names of compounds in MSP-object*

Description

adduct returns adduct ion names of compounds in MSP-object.

Usage

```
adduct(x)
```

Arguments

x object of class MSP

Format

An object of class NULL of length 0.

Value

character

Functions

- adduct: returns adduct ion names of compounds in MSP-objects

Examples

```
data("sd02_deconvoluted", package = "MetCirc")
finalMSP <- convert2MSP(sd02_deconvoluted, split = " _ ",
                        splitIndMZ = 2, splitIndRT = NULL)
adduct(finalMSP)
```

adduct<-

adduct<- sets adduct ion names in MSP-object

Description

adduct<- sets adduct ion names in MSP-object

Arguments

x object of class MSP, see ?convert2MSP for further information
value character vector with new adduct ion names

Format

An object of class NULL of length 0.

Value

MSP-object

Examples

```
data("sd02_deconvoluted", package = "MetCirc")
finalMSP <- convert2MSP(sd02_deconvoluted, split = " _ ",
                        splitIndMZ = 2, splitIndRT = NULL)
adduct(finalMSP) <- rep("Unknown")
```

allocatePrecursor2mz *allocatePrecursor2mz: Join two data sources*

Description

Allocates precursor ions to candidate m / z values based on minimal distance of m / z and deviance of rt based on an objective function

Usage

```
allocatePrecursor2mz(sd01, sd02, kNN = 10, mzCheck = 1, rtCheck = 30,
  mzVsRTbalance = 10000, splitPattern = "_", splitInd = 2)
```

Arguments

sd01	is the output of the XCMS and CAMERA processing and statistical analysis and XCMS and CAMERA scripts (see Li et al. 2015 and vignette for further information)
sd02	data.frame with idMS/MS deconvoluted spectra with fragment ions (m/z, retention time, relative intensity in %) and the corresponding peak correlation group of the precursor ion. sd02 has to have at least four columns: a column 'mz', 'rt', 'intensity' and 'id'
kNN	numerical, number of k-nearest neighbours based on deviation from m/z (i.e. the k entries with the smallest deviation)
mzCheck	numerical, maximum tolerated distance for m/z (strong criterion here)
rtCheck	numerical, maximum tolerated distance for retention time
mzVsRTbalance	numerical, multiplicator for mz value before calculating the (euclidean) distance between two peaks, high value means that there is a strong weight on the deviation m/z value
splitPattern	character, character vector to use for splitting, see ?strsplit for further information
splitInd	numeric, extract precursor mz at position splitInd

Details

This function combines different data sources. `convertExampleDF` is a `data.frame` which comprises information on a specific metabolite per row stating the average retention time, average m/z, the name of the metabolite, the adduct ion name, the spectrum reference file name and additional information (here: TRIO/LVS). `allocatePrecursor2mz` uses `data.frames` of the kind of `sd01_outputXCMS` and `sd02_deconvoluted` to create a `data.frame` of the kind of `convertExampleDF`. Allocation of precursor ions to candidate m/z values is based on minimal distance of m/z and deviance of retention time based on an objective function. We can specify threshold values for m/z and retention time to be used in `allocatePrecursor2mz`, as well as the number of neighbours based on deviation from m/z values. Also, we can specify the weight to base the selection on the m/z compared to the retention time (`mzVsRTbalance`). This might be useful because m/z values might differ less than the retention time in `sd01_outputXCMS` and `sd02_deconvoluted`. Please note, that it might be problematic to compare `sd01_outputXCMS` and `sd02_deconvoluted` and allocate precursor ions therefrom, especially when data were acquired under different conditions.

Value

allocatePrecursor2mz returns a data.frame containing average retention time, average m/z, metabolite name, adduct ion name, spectrum reference

Author(s)

Thomas Naake, <thomasnaake@googlemail.com>

References

Li et al. (2015): Navigating natural variation in herbivory-induced secondary metabolism in coyote tobacco populations using MS/MS structural analysis. PNAS, 112, E4147–E4155, 10.1073/pnas.1503106112.

Examples

```
data("sd01_outputXCMS", package = "MetCirc")
data("sd02_deconvoluted", package = "MetCirc")
data("convertExampleDF", package = "MetCirc")
allocatePrecursor2mz(sd01 = sd01_outputXCMS, sd02 = sd02_deconvoluted,
  kNN = 10, mzCheck = 1, rtCheck = 30, mzVsRTbalance = 10000, splitPattern = " _ ", splitInd = 2)
```

binnedMSP

Example data for MetCirc: binnedMSP

Description

The object binnedMSP is a matrix, where rows are metabolites detected in the tissues sepal (SPL), limb (LIM), anther (ANT) and style (STY). The columns contain binned m/z values. Entries contain the intensity (in percent) of a certain metabolite at a certain m/z value. binnedMSP is derived from the object tissue and compartmentTissue.

Usage

```
binnedMSP
```

Format

```
matrix
```

Value

```
matrix
```

Author(s)

Thomas Naake, <thomasnaake@googlemail.com>

Source

```

data("idMSMStissueproject", package = "MetCirc") data("idMSMStoMSP", package = "MetCirc")
tissueSPL <- compartmentTissue[compartmentTissue[, "SPL"] == TRUE, 1] tissueLIM <- compartmentTissue[compartmentTissue[, "LIM"] == TRUE, 1] tissueANT <- compartmentTissue[compartmentTissue[, "ANT"] == TRUE, 1] tissueSTY <- compartmentTissue[compartmentTissue[, "STY"] == TRUE, 1]

## truncate tissue tissueSPL <- tissue[tissue[,4] tissueLIM <- tissue[tissue[,4] tissueANT <- tissue[tissue[,4] tissueSTY <- tissue[tissue[,4]

## create msp and combine msp objects of different tissues finalMSP <- convert2MSP(tissueSPL, splitIndMZ = 1, splitIndRT = 2, rt = TRUE) finalMSP <- combine(finalMSP, convert2MSP(tissueLIM, splitIndRT = 2, rt = TRUE)) finalMSP <- combine(finalMSP, convert2MSP(tissueANT, splitIndRT = 2, rt = TRUE)) finalMSP <- combine(finalMSP, convert2MSP(tissueSTY, splitIndRT = 2, rt = TRUE))

## create vector with compartments compSPL <- rep("SPL", length(convert2MSP(tissueSPL)))
compLIM <- rep("LIM", length(convert2MSP(tissueLIM))) compANT <- rep("ANT", length(convert2MSP(tissueANT)))
compSTY <- rep("STY", length(convert2MSP(tissueSTY)))

compartment <- c(compSPL, compLIM, compANT, compSTY) binnedMSP <- binning(msp = finalMSP, tol = 0.01, group = compartment, method = "median") save(binnedMSP, file = "binnedMSP.RData", compress = "bzip2")

```

binning

Bin m/z values

Description

Bin m/z values

Usage

```
binning(msp, tol = 0.01, group = NULL, method = c("median", "mean"))
```

Arguments

msp	MSP-object, see ?convert2MSP for further information
tol	numerical, boundary value until which neighbored peaks will be joined together
group	character vector, to which group does the entry belong to
method	character vector, method has to be median or mean

Details

The functions binning bins fragments together by obtaining bins via calculating either mean or medians of fragments which were put in intervals according to the tol parameter.

Value

binning returns a matrix where rownames are precursor ions (m/z / retention time) and colnames are newly calculated m/z values which were binned. Entries are intensity values in

Author(s)

Thomas Naake, <thomasnaake@googlemail.com>

Examples

```
data("idMSMStoMSP", package = "MetCirc")
binning(msp = finalMSP, tol = 0.01, group = NULL, method = "median")
```

cart2Polar

Calculate polar coordinates from cartesian coordinates

Description

cart2Polar calculates polar coordinates from cartesian coordinates

Usage

```
cart2Polar(x, y)
```

Arguments

x	cartesian x coordinate
y	cartesian y coordinate

Details

cart2Polar is employed to translate cartesian coordinates into polar coordinates especially in interactive shiny applications when using hovering and clicking features.

Value

cart2Polar returns a list of polar coordinates r and theta

Author(s)

Thomas Naake, <thomasnaake@googlemail.com>

Examples

```
x <- 1; y <- 1
cart2Polar(x, y)
```

circosLegend	<i>Plot a legend for circos plot</i>
--------------	--------------------------------------

Description

circosLegend plots a legend for circos plot using group names.

Usage

```
circosLegend(groupname, highlight = TRUE, colour = NULL, cex = 1)
```

Arguments

groupname	character vector containing "group" and "name" to display, that is a unique identifier of the features, "group" and "name" have to be separated by "_" where "group" is the first and "name" is the last element
highlight	logical, should colours be adjusted to highlight settings?
colour	NULL or character, colour defines the colours which are used for plotting, if NULL default colours are used
cex	numeric, parameter that controls size of the legend in the plot

Details

Internal use in shinyCircos or outside of shinyCircos to reproduce figures.

Value

The function will open a new plot and display colours together with labels.

Author(s)

Thomas Naake, <thomasnaake@googlemail.com>

Examples

```
## load binnedMSP
data("binnedMSP", package = "MetCirc")
## use only a selection
binnedMSP <- binnedMSP[c(1:20, 29:48, 113:132, 240:259),]
similarityMat <- createSimilarityMatrix(binnedMSP)
groupname <- rownames(similarityMat)
## plot legend
circosLegend(groupname, highlight = TRUE, colour = NULL, cex = 1)
```

classes	<i>classes returns class names of compounds in MSP-object</i>
---------	---

Description

classes returns class names of compounds in MSP-object.

Usage

```
classes(x)
```

Arguments

x object of class MSP

Format

An object of class NULL of length 0.

Value

character

Functions

- classes: returns class names of metabolites in MSP-object

Examples

```
data("sd02_deconvoluted", package = "MetCirc")
finalMSP <- convert2MSP(sd02_deconvoluted, split = " _ ",
                       splitIndMZ = 2, splitIndRT = NULL)
classes(finalMSP)
```

classes<-	<i>classes<- sets information in MSP-object</i>
-----------	--

Description

classes<- sets information in MSP-object.

Arguments

x object of class MSP, see ?convert2MSP for further information
value character vector with new classes

Format

An object of class NULL of length 0.

Value

MSP-object

Examples

```
data("sd02_deconvoluted", package = "MetCirc")
finalMSP <- convert2MSP(sd02_deconvoluted, split = " _ ",
                       splitIndMZ = 2, splitIndRT = NULL)
classes(finalMSP) <- rep("Unknown")
```

combine

combine method for MSP-class

Description

combine combines two objects of class MSP.

Usage

```
combine(object1, object2)
```

```
## S4 method for signature 'MSP,MSP'
combine(object1, object2)
```

Arguments

object1	object of class MSP
object2	object of class MSP

Value

MSP-object

Methods (by class)

- object1 = MSP, object2 = MSP: combines two object of class MSP

Examples

```
data("sd02_deconvoluted", package = "MetCirc")
finalMSP1 <- convert2MSP(sd02_deconvoluted, split = " _ ",
                        splitIndMZ = 2, splitIndRT = NULL)
finalMSP2 <- convert2MSP(sd02_deconvoluted, split = " _ ",
                        splitIndMZ = 2, splitIndRT = NULL)
combine(finalMSP1, finalMSP2)
```

compartmentTissue *Example data for MetCirc: compartmentTissue*

Description

The data.frame compartmentTissue is used in the subsection 'Preparing the tissue data set for analysis' in the vignette of MetCirc. In compartmentTissue, information on the organ-localisation of each MS/MS spectrum is stored.

Usage

```
tissue
```

Format

```
data.frame
```

Value

```
data.frame
```

Author(s)

Thomas Naake, <thomasnaake@googlemail.com>

Source

```
internal
```

convert2MSP *Convert deconvoluted matrix into MSP-object*

Description

Convert deconvoluted matrix into MSP-object

Usage

```
convert2MSP(mm, splitPattern = "_", splitIndMZ = 1, splitIndRT = NULL,
  rt = FALSE, names = FALSE, information = FALSE, classes = FALSE, adduct = FALSE)
```

Arguments

mm	matrix, mm has to have three columns with colnames "mz", "intensity" and "id" (order is not important). The column comprises information about the precursor ion which will be assessed by splitPattern and splitInd. Optionally, mm can have colnames "rt", "names", "information", "classes" and "adduct".
splitPattern	character, splitPattern is the pattern which separates elements and precursor m/z

splitIndMZ	numeric, the position of the precursor m/z in the character string concerning separation by splitPattern
splitIndRT	numeric or NULL, the position of the retention time in the character string concerning separation by splitPattern, if NULL the retention time will be the mean of all retention time values of the MS/MS feature fragments
rt	logical, should retention times be retrieved? If set to TRUE, convert2MSP will access the column "rt" in mm which contains the retention time values for each fragment when splitIndRT is NULL, if rt is set to TRUE and splitIndRT is numeric, convert2MSP will access the column "id" to get the retention time at position splitIndRT when splitting with splitPattern
names	logical, should names be retrieved? If set to TRUE, convert2MSP will access the column "names" in mm which contains the names of the metabolites
information	logical, should further information of metabolites be retrieved? If set to TRUE, convert2MSP will access the column "information" in mm which contains information about the metabolites
classes	logical, should classes of metabolites be retrieved? If set to TRUE, convert2MSP will access the column "classes" in mm which contains the names of the metabolites
adduct	logical, should adduct ion names of metabolites be retrieved? If set to TRUE, convert2MSP will access the column "adduct" in mm which contains the adduct ion names of the metabolites

Details

The function `convert2MSP` creates a data entry for each precursor ion. Each entry in the return object has the following information: Num Peaks and a list of fragments together with their intensities; it will further contain information on m/z values of the precursor ion, the retention time, metabolite names, classes, adduct ion name and further information. `convert2MSP` will access the columns "rt", "names", "information", "classes" and "adduct", respectively, if arguments are set to TRUE. The column "id" has to contain a unique identifier for each MS/MS feature. It is obligatory that each element in the column "id" contains the precursor m/z value, but may contain further elements (e.g. peak correlation value or retention time of the precursor ion). Information about the m/z value will be assessed by `splitPattern` and `splitInd`. E.g. items in the column "id" can be in the form of "1_163.23", which has to be accessed by setting `splitPattern = "_"` and `splitInd = 2` to access the m/z value of the precursor ion (here: 163.23). If `rt` is set to TRUE and `splitIndRT` is NULL, `convert2MSP` will access the column "rt" to get the retention time values corresponding to each fragment and calculate the mean value, if `rt` is set to TRUE and `splitIndRT` numeric, `convert2MSP` will retrieve the retention time value from column "id".

Value

`convert2MSP` returns an object of class MSP

Author(s)

Thomas Naake, <thomasnaake@googlemail.com>

Examples

```
data("sd02_deconvoluted", package = "MetCirc")
convert2MSP(mm = sd02_deconvoluted, splitPattern = "_", splitIndMZ = 2,
  splitIndRT = NULL, rt = FALSE, names = FALSE, information = FALSE,
  classes = FALSE, adduct = FALSE)
```

convertExampleDF	<i>Example data for MetCirc: convertExampleDF</i>
------------------	---

Description

convertExampleDF is a data.frame which comprises information on a specific metabolite per row stating the average retention time, average m/z, the name of the metabolite, the adduct ion name and the spectrum reference file name. The function allocatePrecursor2mz uses data.frames of the kind sd01_outputXCMS and sd02_deconvoluted to create a data.frame of the kind of convertExampleDF. Allocation of precursor ions to candidate m/z values is based on minimal distance of m/z and deviance of retention time based on an objective function. See ?allocatePrecursor2mz for further information.

Usage

```
convertExampleDF
```

Format

```
data.frame
```

Value

```
data.frame
```

Author(s)

```
Thomas Naake, <thomasnaake@gmail.com>
```

Source

```
internal
```

convertMSP2MSP	<i>Convert MSP data frame into object of MSP-class</i>
----------------	--

Description

Convert msp data frame into object of MSP-class

Usage

```
convertMSP2MSP(msp)
```

Arguments

```
msp          data.frame, see Details for further information.
```

Details

msp is a data frame of a .MSP file, a typical data file for MS/MS libraries. The data frame has two columns and contains in the first column the entries "NAME:", "PRECURSORMZ:" (or "EX-ACTMASS:"), "Num Peaks:" and information on fragments and peak areas/intensities. It may additionally contain row entries: convertMSP2MSP will try to find the row entries "RETENTION-TIME:", "ADDUCTIONNAME:" (or "PRECURSORTYPE:"), "CLASS:" and "INFORMATION:" and extract the respective information in the second column.

Value

convertMSP2MSP returns an object of class MSP.

Author(s)

Thomas Naake, <thomasnaake@googlemail.com>

Examples

```
data("convertMSP2MSP", package = "MetCirc")
convertMSP2MSP(msp = msp2msp)
```

createLink0Matrix *Create a link matrix*

Description

Create a link matrix which links every feature in similarity matrix with another.

Usage

```
createLink0Matrix(similarityMatrix)
```

Arguments

similarityMatrix
matrix, a similarity matrix that contains the NDP similarity measure between all precursors in the data set

Details

createLink0Matrix creates a matrix from a similarity matrix which includes all connections between features in the similarity matrix, but exclude links which have a similarity of exactly 0.

Value

createLink0Matrix returns a matrix that gives per each row information on linked features

Author(s)

Thomas Naake, <thomasnaake@googlemail.com>

createOrderedSimMat	<i>Update colnames and rownames of a similarity matrix according to order m/z, retention time and clustering</i>
---------------------	--

Description

Internal function for shiny application. May also be used outside of shiny to reconstruct figures.

Usage

```
createOrderedSimMat(similarityMatrix, order = c("retentionTime", "mz", "clustering"))
```

Arguments

similarityMatrix	matrix, similarityMatrix contains pair-wise similarity coefficients which give information about the similarity between precursors
order	character, one of "retentionTime", "mz" or "clustering"

Details

createOrderSimMat takes a similarity matrix and a character vector as arguments. It will then reorder rows and columns of the similarityMatrix object such, that it orders rows and columns of similarityMatrix according to m/z, retention time or clustering in each group. createOrderSimMat is employed in the shinyCircos function to create similarityMatrix objects which will allow to switch between different types of ordering in between groups (sectors) in the circos plot. It may be used as well externally, to reproduce plots outside of the reactive environment (see vignette for a workflow).

Value

createOrderedSimMat returns a similarity matrix with ordered rownames according to the character vector given to order

Author(s)

Thomas Naake, <thomasnaake@googlemail.com>

Examples

```
data("binnedMSP", package = "MetCirc")
data("similarityMat", package = "MetCirc")
## order according to retention time
createOrderedSimMat(similarityMatrix = similarityMat, order = "retentionTime")
```

```
createSimilarityMatrix
```

Create similarity matrix

Description

Creates the similarity matrix by calculating the normalised dot product (NDP) between precursors

Usage

```
createSimilarityMatrix(mm, m = 0.5, n = 2)
```

Arguments

<code>mm</code>	matrix, colnames are all fragments which occur in the dataset, rownames are m/z / rt values, entries of mm are intensity values corresponding to their m/z values
<code>m</code>	numeric, see ?NDP for further details
<code>n</code>	numeric, see ?NDP for further details

Details

createSimilarityMatrix calls a function to calculate the NDP between all precursors in the data set. For further information on how the NDP is calculated see ?NDP and Li et al. (2015): Navigating natural variation in herbivory-induced secondary metabolism in coyote tobacco populations using MS/MS structural analysis. PNAS, E4147–E4155. Currently $m = 0.5$ and $n = 2$ are set as default.

Value

createSimilarityMatrix returns a similarity matrix that contains the NDP similarity measure between all precursors in the data set

Author(s)

Thomas Naake, <thomasnaake@googlemail.com>

Examples

```
data("binnedMSP", package = "MetCirc")
## truncate binnedMSP
binnedMSP <- binnedMSP[1:28,]
createSimilarityMatrix(binnedMSP, m = 0.5, n = 2)
```

cutLinkMatrix *Create a cut link matrix*

Description

Create a cut link matrix

Usage

```
cutLinkMatrix(LinkMatrix, type = c("all", "inter", "intra"))
```

Arguments

LinkMatrix matrix, that gives per each row information on linked features
type character, one of "all", "inter" or "intra"

Details

This function is used to cut features from LinkMatrix. If type = "all", LinkMatrix will not be changed; if type = "inter" the cut LinkMatrix will only contain entries of links which are between groups and not inside groups; contrary to that, if type = "intra" the cut LinkMatrix will only contain entries of links which are inside groups and not between groups.

Value

cutLinkMatrix returns a matrix that gives per each row information on linked features

Author(s)

Thomas Naake, <thomasnaake@googlemail.com>

Examples

```
data("binnedMSP", package = "MetCirc")  
## use only a selection  
binnedMSP <- binnedMSP[c(c(1:20, 29:48, 113:132, 240:259)),]  
similarityMat <- createSimilarityMatrix(binnedMSP)  
linkMat <- createLinkMatrix(similarityMatrix = similarityMat, threshold_low = 0.75, threshold_high = 1)  
cutLinkMatrix(LinkMatrix = linkMat, type = "all")
```

cutUniquePrecursor *Get unique precursor ions*

Description

Get unique precursor ions

Usage

```
cutUniquePrecursor(precursor, splitPattern = splitPattern,  
                    splitInd = splitInd, returnCharacter = TRUE)
```

Arguments

precursor	character where features are separated by splitPattern
splitPattern	character, character vector to use for splitting, see ?strsplit for further information
splitInd	numeric, extract precursor mz at position splitInd
returnCharacter	logical, if TRUE return character, if FALSE return numeric

Details

Function for internal usage.

Value

The function cutUniquePrecursor returns character or numeric as specified by parameters.

Author(s)

Thomas Naake, <thomasnaake@googlemail.com>

Examples

```
precursor <- "A_269.0455469_-1"
splitPattern <- "_"
splitInd <- 2
cutUniquePrecursor(precursor, splitPattern = splitPattern,
  splitInd = splitInd, returnCharacter = TRUE)
```

getBegEndIndMSP	<i>Get beginning and end indices of each entry in a data.frame in peaks(MSP)-objects</i>
-----------------	--

Description

Get beginning and end indices of each entry in a data.frame in a peaks(MSP)-object

Usage

```
getBegEndIndMSP(msp)
```

Arguments

msp	data.frame in peaks(MSP)-object, see ?convert2MSP for further information
-----	---

Details

Internal use to retrieve start and end row indices for fragments of MS/MS features.

Value

getBegEndIndMSP returns a list of length 2 where the first entry contains the start indices and the second the end indices

Author(s)

Thomas Naake, <thomasnaake@googlemail.com>

Examples

```
data("sd02_deconvoluted", package = "MetCirc")
finalMSP <- convert2MSP(sd02_deconvoluted, split = " _ ",
                       splitIndMZ = 2, splitIndRT = 3)
finalMSPdf <- peaks(finalMSP)
getBegEndIndMSP(finalMSPdf)
```

getLinkMatrixIndices *Get indices in LinkMatrix of feature*

Description

Gets indices in LinkMatrix of feature

Usage

```
getLinkMatrixIndices(groupnameselectd, linkMatrix)
```

Arguments

groupnameselectd

character vector with groupname of selected feature, vector containing "group" and "name" to display, that is a unique identifier of the features, "group" and "name" have to be separated by "_" where "group" is the first and "name" is the last element

linkMatrix matrix, in each row there is information about features to be connected

Details

Internal use for function highlight.

Value

getLinkMatrixIndices returns indices concerning linkMatrix to which groupnameselectd connects

Author(s)

Thomas Naake, <thomasnaake@googlemail.com>

Examples

```
## Not run: getLinkMatrixIndices(groupnameselectd, linkMatrix)
```

getPrecursorMZ	getPrecursorMZ returns precursor m/z values of an MSP-object
----------------	--

Description

getPrecursorMZ returns a numeric vector with precursor m/z values

Usage

```
getPrecursorMZ(x)
```

Arguments

x object of class MSP

Format

An object of class NULL of length 0.

Value

numeric

Functions

- getPrecursorMZ: returns precursor m/z values of an MSP object

Examples

```
data("sd02_deconvoluted", package = "MetCirc")
finalMSP <- convert2MSP(sd02_deconvoluted, split = " _ ",
                       splitIndMZ = 2, splitIndRT = NULL)
getPrecursorMZ(finalMSP)
```

getRT	getRT returns precursor RT values of an MSP-object
-------	--

Description

getRT returns a numeric vector with all retention time values

Usage

```
getRT(x)
```

Arguments

x object of class MSP

Format

An object of class NULL of length 0.

Value

numeric

Functions

- `getRT`: returns precursor RT values of an MSP-object

Examples

```
data("sd02_deconvoluted", package = "MetCirc")
finalMSP <- convert2MSP(sd02_deconvoluted, split = " _ ",
                        splitIndMZ = 2, splitIndRT = NULL)
getRT(finalMSP)
```

highlight

Add links and highlight sectors

Description

A function to add links and highlight sectors to an initialised and plotted circsize plot with one track.

Usage

```
highlight(groupname, ind, LinkMatrix, colour = NULL, transparency = 0.4, links = TRUE)
```

Arguments

groupname	character vector containing "group" and "name" to display, that is a unique identifier of the features, "group" and "name" have to be separated by "_" where "group" is the first and "name" is the last element
ind	numeric, indices which will be highlighted
LinkMatrix	matrix, in each row there is information about features to be connected
colour	NULL or character, colour defines the colours which are used for plotting, if NULL default colours are used
transparency	numeric, defines the transparency of the colours
links	logical, should links of unselected features be plotted

Details

Internal use for shinyCircos or outside of shinyCircos to reproduce the figure.

Value

The function will update an existing plot by highlighting a specified sector and connected links.

Author(s)

Thomas Naake, <thomasnaake@googlemail.com>

Examples

```
## load binnedMSP
data("binnedMSP", package = "MetCirc")
## use only a selection
binnedMSP <- binnedMSP[c(1:20, 29:48, 113:132, 240:259),]
similarityMat <- createSimilarityMatrix(binnedMSP)
## order similarityMat according to retentionTime and update rownames
simM <- createOrderedSimMat(similarityMat, order = "retentionTime")
## create link matrix
linkMat <- createLinkMatrix(similarityMatrix = simM,
  threshold_low = 0.95, threshold_high = 1)
## cut link matrix (here: only display links between groups)
linkMat_cut <- cutLinkMatrix(linkMat, type = "inter")
## set circlize parameters
circos.par(gap.degree = 0, cell.padding = c(0.0, 0, 0.0, 0),
  track.margin = c(0.0, 0))
groupname <- rownames(simM)
## here: set selectedFeatures arbitrarily
indSelected <- c(2,23,42,62)
selectedFeatures <- groupname[indSelected]
## actual plotting
plotCircos(groupname, linkMat_cut, initialize = TRUE,
  featureNames = TRUE, cexFeatureNames = 0.2, groupSector = TRUE,
  groupName = FALSE, links = FALSE, highlight = TRUE)
## highlight
highlight(groupname = groupname, ind = indSelected, LinkMatrix =
  linkMat_cut, colour = NULL, transparency = 0.4, links = TRUE)
```

idMSMStoMSP-data

Example data for MetCirc: finalMSP

Description

finalMSP is of instance MSP, a container for MS/MS data. finalMSP is derived from the object tissue and compartmentTissue.

Usage

```
finalMSP
```

Format

object of class MSP

Value

object of class MSP

Author(s)

Thomas Naake, <thomasnaake@googlemail.com>

Source

```

data("idMSMStissueproject", package = "MetCirc") ## create vectors with precursor names present
in tissue tissueSPL <- compartmentTissue[compartmentTissue,"SPL"] == TRUE, 1] tissueLIM
<- compartmentTissue[compartmentTissue,"LIM"] == TRUE, 1] tissueANT <- compartmentTis-
sue[compartmentTissue,"ANT"] == TRUE, 1] tissueSTY <- compartmentTissue[compartmentTissue,"STY"]
== TRUE, 1]

## truncate tissue tissueSPL <- tissue[tissue[,4] tissueLIM <- tissue[tissue[,4] tissueANT <- tis-
sue[tissue[,4] tissueSTY <- tissue[tissue[,4]

## create msp and combine msp objects of different tissues finalMSP <- convert2MSP(tissueSPL,
rt = TRUE) finalMSP <- combine(finalMSP, convert2MSP(tissueLIM), rt = TRUE) finalMSP <-
combine(finalMSP, convert2MSP(tissueANT), rt = TRUE) finalMSP <- combine(finalMSP, con-
vert2MSP(tissueSTY), rt = TRUE)

## write finalMSP to idMSMStoMSP.RData save(finalMSP, file = "idMSMStoMSP.RData", com-
press = "xz")

```

information

information returns information of metabolites in MSP-object

Description

information returns information in MSP-object.

Usage

```
information(x)
```

Arguments

x object of class MSP, see ?convert2MSP for further information

Format

An object of class NULL of length 0.

Value

character

Functions

- information: returns information of metabolites in MSP-object

Examples

```

data("sd02_deconvoluted", package = "MetCirc")
finalMSP <- convert2MSP(sd02_deconvoluted, split = " _ ",
splitIndMZ = 2, splitIndRT = NULL)
information(finalMSP)

```

```
information<-          information<- sets information in MSP-object
```

Description

information<- sets information in MSP-object

Arguments

x object of class MSP, see ?convert2MSP for further information
value character vector with new information

Format

An object of class NULL of length 0.

Value

MSP-object

Examples

```
data("sd02_deconvoluted", package = "MetCirc")
finalMSP <- convert2MSP(sd02_deconvoluted, split = " _ ",
                        splitIndMZ = 2, splitIndRT = NULL)
information(finalMSP) <- rep("Unknown")
```

```
length                length method for MSP-class
```

Description

Gives the number of entries in the MSP object.

Usage

```
## S4 method for signature 'MSP'
length(x)
```

Arguments

x object of class MSP

Value

numeric

Examples

```
data("sd02_deconvoluted", package = "MetCirc")
finalMSP <- convert2MSP(sd02_deconvoluted, split = " _ ",
                        splitIndMZ = 2, splitIndRT = NULL)
length(finalMSP)
```

minFragCart2Polar	<i>Calculate the nearest feature in polar coordinates given cartesian coordinates</i>
-------------------	---

Description

Calculates the nearest feature in polar coordinates given cartesian coordinates

Usage

```
minFragCart2Polar(x, y, degreeOfFeatures)
```

Arguments

x	cartesian x coordinate
y	cartesian y coordinate
degreeOfFeatures	list of positions of features

Details

minFragCart2Polar is employed to find the feature with the smallest distance from given cartesian coordinates.

Value

minFragCart2Polar returns the index of the feature that has the smallest distance to the given coordinates. As minFragCart2Polar is used in shinyCircos for the track 1 only polar r coordinates between 0.8 and 1 will be used to find the feature with smallest distance.

Author(s)

Thomas Naake, <thomasnaake@gmail.com>

Examples

```
## load binnedMSP
data("binnedMSP", package = "MetCirc")
## use only a selection
binnedMSP <- binnedMSP[c(1:20, 29:48, 113:132, 240:259),]
simM <- createSimilarityMatrix(binnedMSP)
groupname <- rownames(simM)
plotCircos(groupname, NULL, initialize = TRUE, featureNames = FALSE,
            groupName = FALSE, groupSector = FALSE, links = FALSE, highlight = FALSE)
x <- 1
y <- 0
degreeFeatures <- lapply(groupname,
                          function(x) mean(circlize:::get.sector.data(x)[c("start.degree", "end.degree")]))
minFragCart2Polar(x, y, degreeOfFeatures = degreeFeatures)
```

MSP	<i>MSP-class</i>
-----	------------------

Description

Definiton of MSP-class in MetCirc. Entries are MS/MS features including their spectra. Allows easy computation of number of entries by entering `length(msp)`, where `msp` is of class MSP. The MSP-class incorporates accessors for auxiliary information of MS/MS features (names, classes, information, adduct ion name).

Author(s)

Thomas Naake, <thomasnaake@googlemail.com>

`msp2FunctionalLossesMSP`

Convert MSP to MSP with functional losses

Description

`msp2FunctionalLossesMSP` converts a MSP-object (with fragments) into a MSP-object with neutral losses

Usage

```
msp2FunctionalLossesMSP(msp)
```

Arguments

`msp` MSP-object

Details

The function `msp2FunctionalLosses` can be used when calculating the similarity based on neutral losses instead of fragments.

Value

`msp2FunctionalLossesMSP` returns a MSP-object (with neutral losses)

Author(s)

Thomas Naake, <thomasnaake@googlemail.com>

Examples

```
data("sd02_deconvoluted", package = "MetCirc")
finalMSP <- convert2MSP(sd02_deconvoluted, split = "_",
                       splitIndMZ = 2, splitIndRT = NULL)
finalMSPNL <- msp2FunctionalLossesMSP(msp = finalMSP)
```

`msp2msp`*Example data for MetCirc: msp2msp*

Description

`convertMSP2MSP` contains the object `msp2msp` that is a data frame in .MSP format, a typical format for MS/MS library building. Each entry consists of the metabolite name (NAME), the precursor m/z (PRECURSORMZ), the retention time (RETENTIONTIME), number of peaks (Num Peaks), together with fragments and their intensity values. In the example used in the function `convertMSP2MSP` the matrix `msp2msp` is used to construct an object of class MSP.

Usage`msp2msp`**Format**`data.frame`**Value**`data.frame`**Author(s)**

Thomas Naake, <thomasnaake@gmail.com>

Source

http://prime.psc.riken.jp/Metabolomics_Software/MS-DIAL/, truncated .MSP file of GNPS MS/MS Negative (contains 22 entries): http://prime.psc.riken.jp/Metabolomics_Software/MS-DIAL/MSMS-GNPS-Curated-Neg.msp

`names`*names returns names in MSP-object*

Description

`names` returns names in MSP-object.

Usage

```
## S4 method for signature 'MSP'  
names(x)
```

Arguments

`x` object of class MSP, see `?convert2MSP` for further information

Value

character

Examples

```
data("sd02_deconvoluted", package = "MetCirc")
finalMSP <- convert2MSP(sd02_deconvoluted, split = " _ ",
                        splitIndMZ = 2, splitIndRT = NULL)
names(finalMSP)
```

names<-

names<- sets names in MSP-object

Description

names<- sets names in MSP-object

Usage

```
## S4 replacement method for signature 'MSP,character'
names(x) <- value
```

Arguments

x object of class MSP, see ?convert2MSP for further information
value character vector with new names

Value

MSP-object

Examples

```
data("sd02_deconvoluted", package = "MetCirc")
finalMSP <- convert2MSP(sd02_deconvoluted, split = " _ ",
                        splitIndMZ = 2, splitIndRT = NULL)
names(finalMSP) <- rep("Unknown")
```

NDP

Calculate the normalised dot product

Description

Calculate the normalised dot product (NDP)

Usage

```
NDP(matrow1, matrow2, m = 0.5, n = 2, mass)
```

Arguments

matrow1	character or numeric vector, the entries correspond to the mass vector and contain corresponding intensities to the masses, it is the first feature to compare
matrow2	character or numeric vector, the entries correspond to the mass vector and contain corresponding intensities to the masses, it is the second feature to compare
m	numeric, exponent to calculate peak intensity-based weights
n	numeric, exponent to calculate peak intensity-based weights
mass	character or numeric vector, vector with all masses which occur in the data set

Details

The NDP is calculated according to the following formula:

$$NDP = \frac{\sum (W_{S1,i} \cdot W_{S2,i})^2}{\sum (W_{S1,i}^2) * \sum (W_{S2,i}^2)}$$

, with $W = [peakintensity]^m \cdot [m/z]^n$. For further information see Li et al. (2015): Navigating natural variation in herbivory-induced secondary metabolism in coyote tobacco populations using MS/MS structural analysis. PNAS, E4147–E4155. NDP returns a numeric value ranging between 0 and 1, where 0 indicates no similarity between the two MS/MS features, while 1 indicates that the MS/MS features are identical.

Value

NDP returns a numeric similarity coefficient between 0 and 1

Author(s)

Thomas Naake, <thomasnaake@googlemail.com>

Examples

```
data("binnedMSP", package = "MetCirc")
NDP(matrow1 = binnedMSP[1,], matrow2 = binnedMSP[2,], m = 0.5, n = 2,
    mass = colnames(binnedMSP))
```

peaks

peaks *method for MSP-class*

Description

peaks returns the data.frame entry with peak information of an MSP object.

Usage

```
peaks(object)
```

```
## S4 method for signature 'MSP'
peaks(object)
```

Arguments

object object of class MSP

Value

data.frame

Methods (by class)

- MSP: returns the data.frame of an MSP-object

Examples

```
data("sd02_deconvoluted", package = "MetCirc")
finalMSP <- convert2MSP(sd02_deconvoluted, split = "_",
                        splitIndMZ = 2, splitIndRT = NULL)
peaks(finalMSP)
```

plotCircos	<i>Circular plot to visualise similarity</i>
------------	--

Description

Circular plot to visualise similarity

Usage

```
plotCircos(groupname, linkMat, initialize = c(TRUE, FALSE),
           featureNames = c(TRUE, FALSE), cexFeatureNames = 0.3,
           groupSector = c(TRUE, FALSE), groupName = c(TRUE, FALSE),
           links = c(TRUE, FALSE), highlight = c(TRUE, FALSE), colour = NULL,
           transparency = 0.2)
```

Arguments

groupname	character vector containing "group" and "name" to display, that is a unique identifier of the features, "group" and "name" have to be separated by "_" where "group" is the first and "name" is the last element
linkMat	data.frame containing linked features in each row, has five columns (group1, name1, group2, name2, NDP)
initialize	logical, should plot be initialized?
featureNames	logical, should feature names be displayed?
cexFeatureNames	numeric, size of feature names
groupSector	logical, should groups be displayed with background colours?
groupName	logical, should group names (e.g. compartment names or individual names) be displayed?
links	logical, should links be plotted?
highlight	logical, highlight is set to TRUE
colour	NULL or character, colour defines the colours which are used for plotting, if NULL default colours are used
transparency	numeric, defines the transparency of the colours

Details

Internal use for shinyCircos or used outside of shinyCircos to reproduce figure

Value

The function will initialize a circlize plot and/or will plot features of a circlize plot.

Author(s)

Thomas Naake, <thomasnaake@googlemail.com>

Examples

```
## load binnedMSP
data("binnedMSP", package = "MetCirc")
## use only a selection
binnedMSP <- binnedMSP[c(1:20, 29:48, 113:132, 240:259),]
similarityMat <- createSimilarityMatrix(binnedMSP)
## order similarityMat according to retentionTime
simM <- createOrderedSimMat(similarityMat, order = "retentionTime")
## create link matrix
linkMat <- createLinkMatrix(similarityMatrix = simM,
  threshold_low=0.8, threshold_high=1)
## cut link matrix (here: only display links between groups)
linkMat_cut <- cutLinkMatrix(linkMat, type = "inter")
## set circlize paramters
circos.par(gap.degree = 0, cell.padding = c(0.0, 0, 0.0, 0),
  track.margin = c(0.0, 0))
groupname <- rownames(simM)
## actual plotting
plotCircos(groupname, linkMat_cut, initialize = TRUE,
  featureNames = TRUE, cexFeatureNames = 0.3, groupSector = TRUE,
  groupName = FALSE, links = FALSE, highlight = FALSE, colour = NULL,
  transparency = 0.2)
```

printInformationSelect

Display information on connected features of selected features

Description

Displays information on connected features of selected features.

Usage

```
printInformationSelect(groupname, msp = NULL, ind,
  lMatInd, linkMatrixThreshold, similarityMatrix, roundDigits = 2)
```

Arguments

groupname	character vector with groupname of selected feature, vector containing "group" and "name" to display, that is a unique identifier of the features, "group" and "name" have to be separated by "_" where "group" is the first and "name" is the last element
msp	MSP, an S4 object of class MSP for information about the selected feature
ind	numeric
lMatInd	numeric indices of selected features
linkMatrixThreshold	matrix that contains information of linked features for given thresholds
similarityMatrix	matrix that is used to get information on the degree of similarity, similarityMat is an ordered version of a similarity matrix, see ?createOrderedSimMat
roundDigits	numeric, how many digits should be displayed?

Details

printInformationSelect is for internal use.

Value

character that is in HTML format

Author(s)

Thomas Naake, <thomasnaake@googlemail.com>

Examples

```
data("idMSMStoMSP", package = "MetCirc")
data("binnedMSP", package = "MetCirc")
## use only a selection
binnedMSP <- binnedMSP[c(1:20, 29:48, 113:132, 240:259),]
similarityMat <- createSimilarityMatrix(binnedMSP)
groupname <- rownames(similarityMat)
## order similarityMat according to mz
simMat <- createOrderedSimMat(similarityMat, order = "mz")
groupnameMZ <- rownames(simMat)
linkMat_thr <- createLinkMatrix(simMat, 0.8, 1)
ind <- 2
indMZ <- which(groupname[ind] == truncateName(groupnameMZ, NULL, group = TRUE))
linkMatInds <- getLinkMatrixIndices(groupnameMZ[indMZ], linkMat_thr)
MetCirc:::printInformationSelect(groupname = groupname,
  msp = NULL, ind = ind, lMatInd = linkMatInds,
  linkMatrixThreshold = linkMat_thr,
  similarityMatrix = similarityMat, roundDigits = 2)
```

sd01_outputXCMS *Example data for MetCirc: sd01_outputXCMS*

Description

sd01_outputXCMS is the output file from the package XCMS using the data from Li et al. (2015). See Li et al. (2015) for further details.

Usage

sd01_outputXCMS

Format

data.frame

Value

data.frame

Author(s)

Thomas Naake, <thomasnaake@gmail.com>

Source

Li et al. (2015)

sd02_deconvoluted *Example data for MetCirc: sd02_deconvoluted*

Description

sd02_deconvoluted contains MS/MS data from Li et al. (2015). It is a data.frame which hosts m/z values, retention time, intensity and the respective precursor m/z values. sd02_deconvoluted originates from Li et al. (2015). See Li et al. (2015) for further information.

Usage

sd02_deconvoluted

Format

data.frame

Value

data.frame

Author(s)

Thomas Naake, <thomasnaake@googlemail.com>

Source

Li et al. (2015)

shinyCircos

Interactive visualisation of similarity and navigation of MS/MS features

Description

Visualise the similarity of MS/MS features in a reactive context. See Details the vignette for further descriptions on how to use shinyCircos.

Usage

```
shinyCircos(similarityMatrix, msp = NULL, ...)
```

Arguments

similarityMatrix	matrix, similarityMatrix contains pair-wise similarity coefficients which give information about the similarity between MS/MS features
msp	MSP, an S4 object of class MSP, the MSP-object will be used to display information about the selected feature
...	further arguments passed to shinyCircos, e.g. cexFeatureNames to pass to plotCircos to set font size in plotCircos of feature names

Details

The function is based on the shiny and circlize package. The user can choose interactively thresholds, type of links (between or within groups), display information about MS/MS features, permanently select MS/MS features and export selected precursors. When running shinyCircos with the object of class MSP, annotation data of selected MS/MS features will be displayed.

Value

shinyCircos returns a character vector with the (permanently) selected precursors or an object with the entries msp and selectedFeatures if a MSP-object was passed to shinyCircos

Author(s)

Thomas Naake, <thomasnaake@googlemail.com>

Examples

```
data("idMSMStoMSP", package = "MetCirc")
## truncate files
finalMSP <- finalMSP[c(1:20, 29:48, 113:132, 240:259)]
data("binnedMSP", package = "MetCirc")
binnedMSP <- binnedMSP[c(1:20, 29:48, 113:132, 240:259),]
similarityMat <- createSimilarityMatrix(binnedMSP)
## Not run: shinyCircos(similarityMatrix = similarityMat, msp = finalMSP)
```

show	show <i>method for MSP-class</i>
------	----------------------------------

Description

show prints information on the MSP-object (number of entries).

Usage

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

Arguments

object object of class MSP

Value

character

Examples

```
data("sd02_deconvoluted", package = "MetCirc")
finalMSP <- convert2MSP(sd02_deconvoluted, split = " _ ",
                       splitIndMZ = 2, splitIndRT = NULL)
show(finalMSP)
```

similarityMat	<i>Example data for MetCirc: similarityMat</i>
---------------	--

Description

similarityMat is a matrix containing the pair-wise similarity scores derived from the idMSMStissueproject data set. See the vignette for a workflow to reproduce the object similarityMat.

Usage

```
similarityMat
```

Format

matrix

Value

matrix

Author(s)

Thomas Naake, <thomasnaake@googlemail.com>

Source

```
data("binnedMSP", package = "MetCirc") similarityMat <- createSimilarityMatrix(binnedMSP)
save(similarityMat, file = "similarityMat.RData", compress = "xz")
```

thresholdLinkMatrix *Threshold a link matrix*

Description

Threshold a link matrix

Usage

```
thresholdLinkMatrix(linkMatrix, threshold_low, threshold_high)
```

Arguments

linkMatrix	matrix, a link matrix that gives per each row information on linked features
threshold_low	numeric, threshold value for NDP values, below this value linked features will not be returned
threshold_high	numeric, threshold value for NDP values, above this value linked features will not be returned

Details

threshold_low and threshold_high are numerical values and truncates similar/identical precursor ions; similarity is momentarily based on the normalised dot product.

Value

thresholdLinkMatrix returns a matrix that gives per each row information on linked features which are linked above a certain threshold

Author(s)

Thomas Naake, <thomasnaake@googlemail.com>

Examples

```
data("binnedMSP", package = "MetCirc")
## use only a selection
binnedMSP <- binnedMSP[c(c(1:20, 29:48, 113:132, 240:259)),]
similarityMat <- createSimilarityMatrix(binnedMSP)
linkMatrix <- createLinkMatrix(similarityMatrix = similarityMat)
thresholdLinkMatrix(linkMatrix = linkMatrix,
  threshold_low = 0.5, threshold_high=1)
```

tissue	<i>Example data for MetCirc: tissue</i>
--------	---

Description

The `data.frame` `tissue` is used in the subsection 'Preparing the tissue data set for analysis' in the vignette of `MetCirc`. MS/MS data are merged across floral organs in this `data.frame`.

Usage

```
tissue
```

Format

```
data.frame
```

Value

```
data.frame
```

Author(s)

Thomas Naake, <thomasnaake@googlemail.com>

Source

```
internal
```

truncateName	<i>Truncate names</i>
--------------	-----------------------

Description

A function to truncate names

Usage

```
truncateName(groupname, roundDigits = 2, group = FALSE)
```

Arguments

<code>groupname</code>	character vector with group and unique identifier (name)
<code>roundDigits</code>	numeric, how many digits should be displayed?
<code>group</code>	logical, should groups be returned?

Details

`groupname` is a vector of character strings consisting of a group, retention time and m/z value, separated by "_". It is cumbersome to display such long strings. `truncateName` truncates these strings by rounding retention time and m/z values by digits given by `roundDigits`. `truncateName` is an internal function.

Value

truncateName returns groupname with truncated names without group)

Author(s)

Thomas Naake, <thomasnaake@gmail.com>

Examples

```
groupname <- "a_100.12345/10.12345"
truncateName(groupname, roundDigits = 2, group = FALSE)
```

[*Extract parts of a MSP-object*]

Description

[operator acting on an MSP-object to extract parts.

Usage

```
## S4 method for signature 'MSP,numeric'
x[i]
```

Arguments

x	object of class MSP
i	numeric

Value

MSP-object

Examples

```
data("sd02_deconvoluted", package = "MetCirc")
finalMSP <- convert2MSP(sd02_deconvoluted, split = " _ ",
                       splitIndMZ = 2, splitIndRT = NULL)
finalMSP[1]
```

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