### Package ‘MetCirc’

**Type** Package  
**Title** MetCirc - a workflow to analyse and visualise metabolomics data  
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**VignetteBuilder** knitr  
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**biocViews** Metabolomics, MassSpectrometry, Visualization  
**Description** MetCirc comprises a workflow to interactively explore metabolomics data: create MSP, bin m/z values, calculate similarity between precursors and visualise similarities.  
**License** GPL-2  
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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)
allocatePrecursor2mz

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 is a data.frame with dMS/MS deconvoluted spectra with fragment ions (m/z, retention time, relative intensity in %) and the corresponding principal component group with the precursor ion. sd02 has four columns, the first column contains the m/z value, the second column the rt, the third column the intensity, the fourth column the pgroup_precursorMZ

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 (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 therewith, 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, <naake@stud.uni-heidelberg.de>

References

Examples

```r
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

```r
binnedMSP
```

### Format

- `matrix`

### Value

- `matrix`

### Author(s)

Thomas Naake, <naake@stud.uni-heidelberg.de>

### Source

- `internal`

---

binning  
Bin m/z values

### Description

Bin m/z values

### Usage

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

msp  data.frame in msp format, see ?convert2MSP for further information
tol  numerical, boundary value until which neighboured 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 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.

Author(s)

Thomas Naake, <naake@stud.uni-heidelberg.de>

Examples

data(“idMSMStoMSP”, package = “MetCirc”)
##group <- sample(c(“yl”, “ol”, “s”, “r”), size = length(finalMSP), replace=TRUE)
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 colar coordinates r and theta
Author(s)
Thomas Naake, <naake@stud.uni-heidelberg.de>

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

circosLegend

Description
circosLegend plots a legend for circos plot using group names.

Usage
circosLegend(groupname, highlight = c(TRUE, FALSE), colour = NULL)

Arguments
groupname 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

Details
Internal use for shiny app or outside of shiny to reproduce figures.

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

Author(s)
Thomas Naake, <naake@stud.uni-heidelberg.de>

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)
**combine**

*combine method for MSP class*

---

**Description**

Combines two objects of class MSP.

**Usage**

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

```r
## 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 MSP objects

**Examples**

```r
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**

```r
tissue
```
**Format**

data.frame

**Value**

data.frame

**Author(s)**

Thomas Naake, <naake@stud.uni-heidelberg.de>

**Source**

internal

---

**convert2MSP**

Convert deconvoluted matrix into MSP format

**Description**

Convert deconvoluted matrix into MSP format

**Usage**

```r
convert2MSP(mm, splitPattern = "._", splitIndMZ = 1, splitIndRT = 2, names = FALSE, metNames = FALSE, class = FALSE)
```

**Arguments**

- **mm**
  - matrix, mm has to have four columns with colnames mz, rt, intensity (order is not important). In the fourth column there has to information about the precursor ion which will be assessed by splitPattern and splitInd. Optionally, mm can have colnames names, metNames, class.

- **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 in the pcgroup

- **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

- **metNames**
  - logical, should names of metabolites be retrieved? If set to TRUE, convert2MSP will access the column "metNames" in mm which contains the names of the metabolites

- **class**
  - logical, should classes of metabolites be retrieved? If set to TRUE, convert2MSP will access the column "class" in mm which contains the names of the metabolites
Details

Creates a data entry for each precursor ion. Each entry in the return object has the following information: NAME, RETENTIONTIME, PRECURSORMZ, METABOLITENAME, ADDUCTIONNAME, Num Peaks and a list of fragments together with their intensities. convert2MSP will access the column name ‘name’, ‘metNames’ and ‘class’, respectively, if arguments are set to TRUE. In the fourth column there has to be information about the precursor ion which will be assessed by splitPattern and splitInd. E.g. items in the fourth column 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: 162.23).

Value

convert2MSP returns an object of class MSP

Author(s)

Thomas Naake, <naake@stud.uni-heidelberg.de>

Examples

```r
data("sd02_deconvoluted", package = "MetCirc") convert2MSP(mm = sd02_deconvoluted, splitPattern = "_", splitIndMZ = 1, splitIndRT = 2, names = FALSE, metNames = FALSE, class = FALSE)
```

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 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. See ?allocatePrecursor2mz for further information.

Usage

```r
convertExampleDF
```

Format

data.frame

Value

data.frame

Author(s)

Thomas Naake, <naake@stud.uni-heidelberg.de>
createLink0Matrix

Source

internal

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 similarityMatrix which includes all connections between features in the similarityMatrix, 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, <naake@stud.uni-heidelberg.de>

Examples

data("binnedMSP", package = "MetCirc")
## truncate binnedMSP
binnedMSP <- binnedMSP[1:28,]
namesPrec <- rownames(binnedMSP)
similarityMat <- createSimilarityMatrix(binnedMSP)
link0Mat <- createLink0Matrix(similarityMatrix = similarityMat)
createLinkMatrix

Create a matrix which contains features to link (indices)

Description
Create a matrix which contains features to link (indices)

Usage
createLinkMatrix(similarityMatrix, threshold)

Arguments
- similarityMatrix: matrix, a similarity matrix that contains the NDP similarity measure between all precursors in the data set
- threshold: numerical, threshold value for NDP values, below this value linked features will not be included

Details
threshold is a numerical value and filters linked precursor ions; filtering is currently based on the normalised dot product.

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

Author(s)
Thomas Naake, <naake@stud.uni-heidelberg.de>

Examples
data("binnedMSP", package = "MetCirc")
## use only a selection
similarityMat <- createSimilarityMatrix(binnedMSP)
createLinkMatrix(similarityMatrix = similarityMat, threshold = 0.5)

createOrderedSimMat

Update colnames and rownames of a similarity matrix according to order m/z, retention time and clustering

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

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

Description

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

Usage

createSimilarityMatrix(mm)

Arguments

mm matrix, colnames are all fragments which occur in the dataset, rownames are m/z / rt values, entries of mm are intensity values corresponding to the mass
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.

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

Author(s)
Thomas Naake, <naake@stud.uni-heidelberg.de>

Examples
data("binnedMSP", package = "MetCirc")
## truncate binnedMSP
binnedMSP <- binnedMSP[1:28,]
createSimilarityMatrix(binnedMSP)

______________________________________________
cutLinkMatrix  Create a cut LinkMatrix

Description
Create a cut LinkMatrix

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, <naake@stud.uni-heidelberg.de>
Examples

data("binnedMSP", package = "MetCirc")
## use only a selection
binnedMSP <- binnedMSP[c(1:20, 29:48, 113:132, 240:259),]
similarityMat <- createSimilarityMatrix(binnedMSP)
linkMat <- createLinkMatrix(similarityMatrix = similarityMat, threshold = 0.5)
cutLinkMatrix(LinkMatrix = linkMat, type = "all")

cutUniquePreMZ Get unique precursor ions

Description

Get unique precursor ions

Usage

cutUniquePreMZ(precursor, splitPattern = splitPattern,
               splitInd = splitInd, returnCharacter = TRUE)

Arguments

precursor, character with 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

Internal function.

Value

cutUniquePreMZ returns character as specified by parameters

Author(s)

Thomas Naake, <naake@stud.uni-heidelberg.de>

Examples

## Not run: cutUniquePreMZ(precursor, splitPattern = splitPattern,
## splitInd = splitInd, returnCharacter = TRUE)
## End(Not run)
getBegEndIndMSP

Get beginning and end indices of each entry in a data.frame in msp format

Description
Get beginning and end indices of each entry in a data.frame in msp format

Usage
getBegEndIndMSP(msp)

Arguments
msp data.frame in msp format, see ?convert2MSP for further information

Details
Internal use to retrieve indices when fragments start and end.

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, <naake@stud.uni-heidelberg.de>

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

getLinkMatrixIndices
Get indices in LinkMatrix of feature

Description
Gets indices in LinkMatrix of feature

Usage
getLinkMatrixIndices(groupnameselected, linkMatrix)
Arguments

groupnameselected
   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 groupnameselected connects

Author(s)

Thomas Naake, <naake@stud.uni-heidelberg.de>

Examples

## Not run: getLinkMatrixIndices(groupnameselected, linkMatrix)

---

getMetaboliteClass returns names of compounds in MSP object

Description

getMetaboliteClass returns names of compounds in MSP object.

Usage

getMetaboliteClass(object)

Arguments

object
   object of class MSP

Format

An object of class NULL of length 0.

Value

character

Functions

- getMetaboliteClass: returns class names of compounds in MSP objects
**getMetaboliteName**

Examples

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

**Description**

getMetaboliteName returns names in MSP object.

**Usage**

```r
getMetaboliteName(object)
```

**Arguments**

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

**Format**

An object of class `NULL` of length 0.

**Value**

character

**Functions**

- `getMetaboliteName`: returns names of metabolites in MSP objects

**Examples**

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

getMSP method for MSP class

Description

Returns the data.frame entry of an MSP object.

Usage

getMSP(object)

## S4 method for signature 'MSP'
getMSP(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)
getMSP(finalMSP)

getName

getName returns names in MSP object

Description

getName returns names in MSP object.

Usage

getName(object)

Arguments

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

Format

An object of class NULL of length 0.
getPrecursorMZ

Value

character

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)
getName(finalMSP)

getPrecursorMZ

getPrecursorMZ returns precursor m/z values of an MSP object

Description

genericPrecursorMZ returns a numeric vector with precursor m/z values

Usage

genericPrecursorMZ(object)

Arguments

object: 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**

```r
getRT(object)
```

**Arguments**

- `object`: 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**

```r
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 circlize plot with one track.

**Usage**

```r
highlight(groupname, ind, LinkMatrix, colour = NULL, transparency = 0.4)
```
 Arguments  

- **groupname**: 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**: numerical, 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**: numerical, defines the transparency of the colours.

 Details

- Internal use for shiny app.

 Value

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

 Author(s)

- Thomas Naake, <naake@stud.uni-heidelberg.de>

 Examples

```r
## 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=0.95)
## 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))
## 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)
```
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, <naake@stud.uni-heidelberg.de>

**Source**

internal

---

**length**

**length method for MSP class**

**Description**

Gives the number of entries in the MSP object.

**Usage**

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

**Arguments**

- `x` object of class MSP

**Value**

numerical
**Examples**

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

**minFragCart2Polar**

Calculate the nearest feature in polar coordinates given cartesian coordinates

**Description**

Calculates the nearest feature in polar coordinates given cartesian coordinates

**Usage**

```r
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, <naake@stud.uni-heidelberg.de>

**Examples**

```r
## load binnedMSP
data("binnedMSP", package = "MetCirc")
## use only a selection
binnedMSP <- binnedMSP[c(1:20, 29:48, 113:132, 240:259),]
simM <- createSimilarityMatrix(binnedMSP)
grouname <- rownames(simM)
plotCircos(grouname, 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**

** MSP-class **

**Description**

MSP class for msp data.frame. Allows easy computation of length of entries by entering length(msp), where msp is of class MSP.

**Arguments**

msp  

a data.frame in msp format

**Author(s)**

Thomas Naake, <naake@stud.uni-heidelberg.de>

---

**msp2FunctionalLossesMSP**

* Convert MSP to MSP with functional losses

**Description**

msp2FunctionalLossesMSP converts a data.frame in msp format (with fragments) into a data.frame in msp format (with neutral losses)

**Usage**

msp2FunctionalLossesMSP(msp)

**Arguments**

msp  

data.frame, a data.frame in msp format (with fragments)

**Details**

msp2FunctionalLosses can be used when you want to calculate the similarity based on neutral losses instead of fragments

**Value**

msp2FunctionalLossesMSP returns a data.frame in msp format (with neutral losses).

**Author(s)**

Thomas Naake, <naake@stud.uni-heidelberg.de>
Examples

```r
## Not run: msp2FunctionalLossesMSP(msp)
data("sd02_deconvoluted", package = "MetCirc")
finalMSP <- convert2MSP(sd02_deconvoluted, split = " _ ",
                        splitIndMZ = 2, splitIndRT = NULL)
finalMSPNL <- msp2FunctionalLossesMSP(msp = finalMSP)
```

NDP

*Calculate the normalised dot product*

**Description**

Calculate the normalised dot product (NDP)

**Usage**

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

**Arguments**

- `matrow1`: character vector or numerical vector, the entries correspond to the mass vector and contain corresponding intensities to the masses, it is the first feature to compare
- `matrow2`: character vector or numerical 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 vector or numerical vector, vector with all masses which occur in the data set

**Details**

The NDP is calculated according to the following formula:

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

, with $W = [\text{peakintensity}]^m \cdot [m/z]^n$. 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 precursors, while 1 indicates a strong similarity between the two precursors.

**Value**

NDP returns a numeric similarity coefficient between 0 and 1

**Author(s)**

Thomas Naake, <naake@stud.uni-heidelberg.de>
Examples

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

plotCircos
Circular plot to visualise similarity

Description
Circular plot to visualise similarity

Usage

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

Arguments

groupName  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 numerical, 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, are we in highlighting mode?
colour      NULL or character, colour defines the colours which are used for plotting; if NULL default colours are used
transparency numerical, defines the transparency of the colours

Details
Internal use for shiny app

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

Display information on connected features of hovered features

Description

Displays information on connected features of hovered features.

Usage

printInformationHover(groupname, msp = NULL, ind, lMatIndHover, linkMatrixThreshold, similarityMatrix)

Arguments

- **groupname**: 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 hovered feature
- **ind**: numeric
- **lMatIndHover**: numeric indices of connected features
- **linkMatrixThreshold**: matrix that contains information of linked features of a threshold or greater
- **similarityMatrix**: matrix that is used to get information on the degree of similarity, similarityMat is an ordered version of a similarity matrix

Examples

```r
## load binnedMSP
data("binnedMSP", package = "MetCirc")

## use only a selection
similarityMat <- createSimilarityMatrix(binnedMSP)

## order similarityMat according to retentionTime
simM <- createOrderedSimMat(similarityMat, order = "retentionTime")

## create link matrix
linkMat <- createLinkMatrix(similarityMatrix = simM, threshold = 0.8)

## 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, 0.0),
           track.margin = c(0.0, 0.0))
groupname <- rownames(simM)

## actual plotting
plotCircos(groupname, linkMat_cut, initialize = TRUE,
           featureNames = TRUE, cexFeatureNames = 0.2, groupSector = TRUE,
           groupName = FALSE, links = FALSE, highlight = FALSE, colour = NULL,
           transparency = 0.2)
```
Details

printInformationHover is for internal use.

Value

character that is in HTML format

Author(s)

Thomas Naake, <naake@stud.uni-heidelberg.de>

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)
## order similarityMat according to mz
simMat <- createOrderedSimMat(similarityMat, order = "mz")
groupname <- rownames(simMat)
linkMat_thr <- createLinkMatrix(simMat, 0.9)
ind <- 19
linkMatIndsHover <- getLinkMatrixIndices(groupname[ind], linkMatThr)
MetCirc:::printInformationHover(groupname = groupname, 
msp = NULL, ind = ind, lMatIndHover = linkMatIndsHover, 
linkMatrixThreshold = linkMat_thr, 
similarityMatrix = simMat)

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, <naake@stud.uni-heidelberg.de>
sd02_deconvoluted

**Source**
Li et al. (2015)

**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, <naake@stud.uni-heidelberg.de>

**Source**

Li et al. (2015)

---

setMetaboliteClass

**setMetaboliteClass sets class names of compounds in MSP objects**

**Description**

setMetaboliteClass sets names of class names of compounds in MSP objects. To set names pass a vector with class names to the argument class.

**Usage**

setMetaboliteClass(object, class)

**Arguments**

<table>
<thead>
<tr>
<th>Name</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>object</td>
<td>object of class MSP</td>
</tr>
<tr>
<td>class</td>
<td>character, a vector with new class names</td>
</tr>
</tbody>
</table>
setMetaboliteName

Format
An object of class NULL of length 0.

Value
MSP

Functions
• setMetaboliteName: sets metabolite names in MSP objects

Examples
data("sd02_deconvoluted", package = "MetCirc")
finalMSP <- convert2MSP(sd02_deconvoluted, split = "_ ",
               splitIndMZ = 2, splitIndRT = NULL)
setMetaboliteClass(finalMSP, c(rep("unknown", 359), "class1"))

setMetaboliteName setMetaboliteName sets metabolite names in MSP objects

Description
setMetaboliteName sets metabolite names in MSP objects. To set metabolite names pass a vector with names to the argument class.

Usage
setMetaboliteName(object, metName)

Arguments
object object of class MSP
metName character, a vector with new metabolite names

Format
An object of class NULL of length 0.

Value
MSP

Functions
• setMetaboliteName: sets metabolite names in MSP objects

Examples
data("sd02_deconvoluted", package = "MetCirc")
finalMSP <- convert2MSP(sd02_deconvoluted, split = "_ ",
               splitIndMZ = 2, splitIndRT = NULL)
setMetaboliteName(finalMSP, c(rep("unknown", 358), "met1", "met2"))
setName

setName sets names in MSP objects

Description

setName sets names in MSP objects. To set names pass a vector with names to the argument class.

Usage

setName(object, name)

Arguments

object object of class MSP
name character, a vector with new names

Format

An object of class NULL of length 0.

Value

MSP

Functions

• setName: sets names in MSP objects

Examples

data("sd02_deconvoluted", package = "MetCirc")
finalMSP <- convert2MSP(sd02_deconvoluted, split = "-_ ",
splitIndMZ = 2, splitIndRT = NULL)
setMetaboliteName(finalMSP, c(rep("unknown", 358), "name1", "name2"))

shinyCircos

Interactive visualisation of similar precursors

Description

Visualise similar precursors.

Usage

shinyCircos(similarityMatrix, msp, size = 400)
show

Arguments

similarityMatrix
matrix, similarityMatrix contains pair-wise similarity coefficients which give
information about the similarity between precursors

msp
MSP, an S4 object of class ‘MSP’ for information about the hovered feature

size
numerical, image width/height in pixels

Details
The function is based on the shiny and circlize package. Choose interactively thresholds, type of
links, hover over precursors, select precursors.

Value

shinyCircos returns a character vector with the selected precursors

Author(s)

Thomas Naake, <naake@stud.uni-heidelberg.de>

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(similarityMat, finalMSP, size = 400)

show

Description
Prints information on the MSP class (number of entries).

Usage

## S4 method for signature ‘MSP’
show(object)

Arguments

object object of class MSP

Value

character
Examples

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

---

**similarityMat**

*Example data for MetCirc: similarityMat*

**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, <naake@stud.uni-heidelberg.de>

**Source**

internal

---

**thresholdLinkMatrix**

*Threshold a link matrix*

**Description**

Threshold a link matrix

**Usage**

`thresholdLinkMatrix(linkMatrix, threshold)`

**Arguments**

- `linkMatrix` : matrix, a link matrix that gives per each row information on linked features
- `threshold` : numerical, threshold value for NDP values, below this value linked features will not be returned
Details

treshold is a numerical value and filters linked precursor ions; filtering is currently 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, <naake@stud.uni-heidelberg.de>

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 <- createLink0Matrix(similarityMatrix = similarityMat)
thresholdLinkMatrix(linkMatrix = linkMatrix, threshold = 0.5)

tissue

Example data for MetCirc: tissue

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, <naake@stud.uni-heidelberg.de>

Source

internal
### Description

A function to truncate names

### Usage

`truncateName(groupname, roundDigits = 2)`

### Arguments

- **groupname**: vector with group and unique identifier (name)
- **roundDigits**: numeric, how many digits should be displayed?

### 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, <naake@stud.uni-heidelberg.de>

### Examples

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

### Extract parts of a MSP object

[ operator acting on an MSP object to extract parts.

### Usage

```r
# S4 method for signature 'MSP,numeric,missing,missing'
x[i, j = "missing",
    drop = "missing"]
```
Arguments

- **x**: object of class MSP
- **i**: numeric
- **j**: missing
- **drop**: missing

Value

MSP object

Examples

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