Package ‘MetCirc’

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Type Package

Title A workflow to analyse and visualise 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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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.

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R topics documented:

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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 idMS/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 m/z 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 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

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

internal

binning

Bin m/z values

Description

Bin m/z values

Usage

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, <thomasnaake@googlemail.com>

**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
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.

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)
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,<thomasnaake@googlemail.com>

Source
internal

convert2MSP  Convert deconvoluted matrix into MSP format

Description
Convert deconvoluted matrix into MSP format

Usage
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 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, <thomasnaake@googlemail.com>

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

convertExampleDF

Format

data.frame

Value

data.frame

Author(s)

Thomas Naake, <thomasnaake@googlemail.com>
createLink0Matrix

Source

internal

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, <thomasnaake@googlemail.com>

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**

```r
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, <thomasnaake@googlemail.com>

**Examples**

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

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

Create similarity matrix

Description

Creates the 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

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 used 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 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, <thomasnaake@googlemail.com>

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, <thomasnaake@googlemail.com>
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, <thomasnaake@googlemail.com>

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, <thomasnaake@googlemail.com>

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)
getMetaboliteClass

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, <thomasnaake@googlemail.com>

Examples

## Not run: getLinkMatrixIndices(groupnameselected, linkMatrix)

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

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

getMetaboliteName

getMetaboliteName returns names of metabolites in MSP object

Description

getMetaboliteName returns names in MSP object.

Usage

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

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**

```r
getMSP(object)
```

```r
## 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**

```r
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**

```r
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

- `getName`: returns names in MSP objects

Examples

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

Description

gPrecursorMZ returns precursor m/z values of an MSP object

Usage

gPrecursorMZ(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

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

getRT returns precursor RT values of an MSP object

Description
getRT returns a numeric vector with all retention time values

Usage
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

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
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, <thomasnaake@googlemail.com>

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))
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)
```
**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**

internal

**length**

**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

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

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@googlemail.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)
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

<table>
<thead>
<tr>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>MSP class for msp data.frame. Allows easy computation of length of entries by entering length(msp), where msp is of class MSP.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Arguments</th>
</tr>
</thead>
<tbody>
<tr>
<td>msp: a data.frame in msp format</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Author(s)</th>
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<tbody>
<tr>
<td>Thomas Naake, <a href="mailto:thomasnaake@googlemail.com">thomasnaake@googlemail.com</a></td>
</tr>
</tbody>
</table>

### msp2FunctionalLossesMSP

*Convert MSP to MSP with functional losses*

<table>
<thead>
<tr>
<th>Description</th>
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<tbody>
<tr>
<td>msp2FunctionalLossesMSP converts a data.frame in msp format (with fragments) into a data.frame in msp format (with neutral losses)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Usage</th>
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</thead>
<tbody>
<tr>
<td>msp2FunctionalLossesMSP(msp)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Arguments</th>
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</thead>
<tbody>
<tr>
<td>msp: data.frame, a data.frame in msp format (with fragments)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Details</th>
</tr>
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<tbody>
<tr>
<td>msp2FunctionalLosses can be used when you want to calculate the similarity based on neutral losses instead of fragments</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Value</th>
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<tbody>
<tr>
<td>msp2FunctionalLossesMSP returns a data.frame in msp format (with neutral losses).</td>
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</table>

<table>
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<tr>
<th>Author(s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thomas Naake, <a href="mailto:thomasnaake@googlemail.com">thomasnaake@googlemail.com</a></td>
</tr>
</tbody>
</table>
## 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**

`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, <thomasnaake@googlemail.com>
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

grouname 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.
### Examples

```r
## load binnedMSP
data("binnedMSP", package = "MetCirc")
## use only a selection
binnedMSP <- binnedMSP[c(1:20, 29:48), ]
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 circclize parameters
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 = 0.2, groupSector = TRUE,
       groupName = FALSE, links = FALSE, highlight = FALSE, colour = NULL, 
       transparency = 0.2)
```

### Description

Displays information on connected features of hovered features.

### Usage

```r
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
Details

printInformationHover 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)
## 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], linkMat_thr)
MetCirc:::printInformationHover(groupname = groupname,
msp = NULL, ind = ind, lMatIndHover = linkMatIndsHover,
linkMatrixThreshold = linkMat_thr,
similarityMatrix = simMat)

data.frame

data.frame

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@googlemail.com>
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, <thomasnaake@googlemail.com>

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

Format
An object of class NULL of length 0.

Value
MSP

Functions
- setMetaboliteClass: sets class names of compounds in MSP objects

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

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

Usage
```r
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
```r
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)
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, <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(similarityMat, finalMSP, size = 400)

Description

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

Usage

```r
## 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)

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

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

threshold 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,<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 <- 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,<thomasnaake@googlemail.com>

Source

internal
**truncateName**

**Truncate names**

**Description**
A function to truncate names

**Usage**

```r
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, <thomasnaake@googlemail.com>

**Examples**

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

```
[  Extract parts of a MSP object
```

**Description**

[ 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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