Package ‘MetCirc’

January 31, 2017

Type Package
Title A workflow to analyse and visualise metabolomics data
Version 1.0.1
Date 2016-12-20
Author Thomas Naake <thomasnaake@googlemail.com> and Emmanuel Gaquerel
     <emmanuel.gaquerel@cos.uni-heidelberg.de>
Maintainer Thomas Naake <thomasnaake@googlemail.com>
VignetteBuilder knitr
Depends R (>= 3.3), amap (>= 0.8), circlize (>= 0.3.5), graphics (>= 3.3),
       grDevices (>= 3.3), methods (>= 3.3), scales (>= 0.3.0),
       shiny (>= 0.13.1), stats (>= 3.3)
Suggests BiocGenerics, knitr (>= 1.11)
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
RoxygenNote 5.0.1
NeedsCompilation no

R topics documented:

  allocatePrecursor2mz ........................................ 2
  binnedMSP .................................................. 4
  binning ..................................................... 4
  cart2Polar .................................................. 5
  circosLegend ............................................... 6
  combine ...................................................... 7
  compartmentTissue ................................ .......... 7
  convert2MSP ................................................ 8
  convertExampleDF .......................................... 9
  createLink0Matrix ......................................... 10
  createLinkMatrix ........................................ 11
  createOrderedSimMat ....................................... 11
  createSimilarityMatrix .................................... 12
allocatePrecursor2mz

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

Usage

```r
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).

ds02 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 pgroupPrecursorMZ.

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 deviancy 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"))
**cart2Polar**

**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**

```r
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**

```r
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

Author(s)

Thomas Naake, <thomasnaake@googlemail.com>

Examples

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

circosLegend

Plot a legend for circos plot

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, <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)
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
```
**convert2MSP**

**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 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, <thomasnaake@googlemail.com>

Examples

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

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, <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

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

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

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
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, <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>
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 infor-
mation
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)

---

getMetaboliteClass

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

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

gMetaboliteName

gMetaboliteName returns names of metabolites in MSP object

Description

gMetaboliteName returns names in MSP object.

Usage

gMetaboliteName(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**

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)
geMSP(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

• getName: returns names in MSP objects

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

getPrecursorMZ returns a numeric vector with precursor m/z values

Usage

getPrecursorMZ(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

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)
```
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 compartment tissue.

Usage

finalMSP

Format

object of class MSP

Value

object of class MSP

Author(s)

Thomas Naake, <thomasnaake@googlemail.com>

Source

internal

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

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**

```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)
grouopname <- rownames(simM)
plotCircos(groupname, NULL, initialize = TRUE, featureNames = FALSE,
            groupName = FALSE, groupSector = FALSE, links = FALSE, highlight = FALSE)
x <- 1
y <- 0
```
MSP

**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, <thomasnaake@googlemail.com>

---

**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**

`msp2FunctionalLossesMSP` 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, <thomasnaake@googlemail.com>
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:

\[ NDP = \frac{\sum (W_{S1,i} \cdot W_{S2,i})^2}{\sum W^2_{S1,i} \cdot \sum W^2_{S2,i}} \]

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 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>
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.
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
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),
track.margin = c(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)
```

printInformationHover  Display information on connected features of hovered features

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)

sd01_outputXCMS

Example data for MetCirc: sd01_outputXCMS

Description

ds01_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"))
```

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
```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**

```r
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

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

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)
Examples

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, <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[cb(c(c(1:20, 29:48, 113:132, 240:259))],]
similarityMat <- createSimilarityMatrix(binnedMSP)
linkMatrix <- createLinkMatrix(similarityMatrix = similarityMat)
thresholdLinkMatrix(linkMatrix = linkMatrix, threshold = 0.5)

---

<table>
<thead>
<tr>
<th>tissue</th>
<th>Example data for MetCirc: tissue</th>
</tr>
</thead>
</table>

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**

**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, <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]
Index

topic datasets
getMetaboliteClass, 16
getMetaboliteName, 17
getName, 18
getPrecursorMZ, 19
getRT, 20
setMetaboliteClass, 29
setMetaboliteName, 30
setName, 31
[ , 35
[,MSP,numeric,missing,missing-method (]), 35
allocatePrecursor2mz, 2
binnedMSP, 4
binning, 4
cart2Polar, 5
circosLegend, 6
combine, 7
combine,MSP,MSP-method (combine), 7
combine,MSP-method (combine), 7
compartmentTissue, 7
convert2MSP, 8
convertExampleDF, 9
createLink0Matrix, 10
createLinkMatrix, 11
createOrderedSimMat, 11
createSimilarityMatrix, 12
cutLinkMatrix, 13
cutUniquePreMZ, 14
finalMSP (idMSSMstoMSP-data), 22
getBegEndIndMSP, 15
getLinkMatrixIndices, 15
getMetaboliteClass, 16
getMetaboliteClass,MSP-method (getMetaboliteClass), 16
getMetaboliteName, 17
getMetaboliteName,MSP-method (getMetaboliteName), 17
getMSP, 18
getMSP,MSP-method (getMSP), 18
getName, 18
getName,MSP-method (getName), 18
getPrecursorMZ, 19
getPrecursorMZ,MSP-method (getPrecursorMZ), 19
getRT, 20
getRT,MSP-method (getRT), 20
highlight, 20
idMSSMstoMSP-data, 22
length, 22
length,MSP-method (length), 22
minFragCart2Polar, 23
MSP, 24
MSP-class (MSP), 24
msp2FunctionalLossesMSP, 24
NDP, 25
plotCircos, 26
printInformationHover, 27
sd01_outputXCMS, 28
sd02_deconvoluted, 29
setMetaboliteClass, 29
setMetaboliteClass,character,MSP-method (setMetaboliteClass), 29
setMetaboliteName, 30
setMetaboliteName,character,MSP-method (setMetaboliteName), 30
setName, 31
setName,character,MSP-method (setName), 31
shinyCircos, 31
show, 32
show,MSP-method (show), 32
similarityMat, 33
thresholdLinkMatrix, 33
tissue, 34
truncateName, 35