Package 'pmd'

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Type Package

Title Paired Mass Distance Analysis for GC/LC-MS Based Non-Targeted Analysis and Reactomics Analysis

Version 0.2.7

Description Paired mass distance (PMD) analysis proposed in Yu, Olkowicz and Pawliszyn (2018) <doi:10.1016/j.aca.2018.10.062> and PMD based reactomics analysis proposed in Yu and Petrick (2020) <doi:10.1038/s42004-020-00403-z> for gas/liquid chromatography–mass spectrometry (GC/LC-MS) based non-targeted analysis. PMD analysis including GlobalStd algorithm and structure/reaction directed analysis. GlobalStd algorithm could found independent peaks in m/z-retention time profiles based on retention time hierarchical cluster analysis and frequency analysis of paired mass distances within retention time groups. Structure directed analysis could be used to find potential relationship among those independent peaks in different retention time groups based on frequency of paired mass distances. Reactomics analysis could also be performed to build PMD network, assign sources and make biomarker reaction discovery. GUIs for PMD analysis is also included as 'shiny' applications.

URL https://yufree.github.io/pmd/

BugReports https://github.com/yufree/pmd/issues

License GPL-2

Encoding UTF-8

LazyData true

Suggests knitr, shiny, rmarkdown

VignetteBuilder knitr

Depends R (>= 3.5.0)

Imports RColorBrewer, stats, graphics, utils, igraph, enviGCMS

RoxygenNote 7.3.2

NeedsCompilation no

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Contents

`getcda` *Perform correlation directed analysis for peaks list.*

Description

Perform correlation directed analysis for peaks list.

Usage

```
getcda(list, corcutoff = 0.9, rtcutoff = 10, accuracy = 4)
```

Arguments

list	a list with mzrt profile
corcutoff	cutoff of the correlation coefficient, default NULL
rtcutoff	cutoff of the distances in retention time hierarchical clustering analysis, default 10
accuracy	measured mass or mass to charge ratio in digits, default 4

Value

list with correlation directed analysis results

See Also

getsda,getrda

Examples

```
data(spmeinvivo)
cluster <- getcorcluster(spmeinvivo)
cbp <- enviGCMS::getfilter(cluster,rowindex = cluster$stdmassindex2)
cda <- getcda(cbp)
```

---

getchain *Get reaction chain for specific mass to charge ratio*

Description

Get reaction chain for specific mass to charge ratio

Usage

```
getchain(
  list,
  diff,
  mass,
  digits = 2,
  accuracy = 4,
  rtcutoff = 10,
  corcutoff = 0.6,
  ppm = 25
)
```

Arguments

list	a list with mzrt profile
diff	paired mass distance(s) of interests
mass	a specific mass for known compound or a vector of masses. You could also input formula for certain compounds
digits	mass or mass to charge ratio accuracy for pmd, default 2
accuracy	measured mass or mass to charge ratio in digits, default 4
rtcutoff	cutoff of the distances in retention time hierarchical clustering analysis, default 10
corcutoff	cutoff of the correlation coefficient, default 0.6
ppm	all the peaks within this mass accuracy as seed mass or formula

Value

a list with mzrt profile and reaction chain dataframe

Examples

```
data(spmeinvivo)
# check metabolites of C18H39NO
pmd <- getchain(spmeinvivo,diff = c(2.02,14.02,15.99),mass = 286.3101)
# remove the retention time for mass only data
spmeinvivo$rt <- NULL
pmd <- getchain(spmeinvivo,diff = c(2.02,14.02,15.99),mass = 286.3101)
```

---

getcluster *Get Pseudo-Spectrum as peaks cluster based on pmd analysis.*

Description

Get Pseudo-Spectrum as peaks cluster based on pmd analysis.

Usage

```
getcluster(list, corcutoff = NULL, accuracy = 4)
```

Arguments

list	a list from getstd function
corcutoff	cutoff of the correlation coefficient, default NULL
accuracy	measured mass or mass to charge ratio in digits, default 4

Value

list with Pseudo-Spectrum index

See Also

getpaired,getstd,plotstd

Examples

```
data(spmeinvivo)
re <- getpaired(spmeinvivo)
re <- getstd(re)
cluster <- getcluster(re)
```

---

getcorcluster *Get Pseudo-Spectrum as peaks cluster based on correlation analysis.*

Description

Get Pseudo-Spectrum as peaks cluster based on correlation analysis.

Usage

```
getcorcluster(list, corcutoff = 0.9, rtcutoff = 10, accuracy = 4)
```

Arguments

list	a list with peaks intensity
corcutoff	cutoff of the correlation coefficient, default 0.9
rtcutoff	cutoff of the distances in cluster, default 10
accuracy	measured mass or mass to charge ratio in digits, default 4

Value

list with Pseudo-Spectrum index

Examples

```
data(spmeinvivo)
cluster <- getcorcluster(spmeinvivo)
```

getms2pmd *read in MSP file as list for ms/ms annotation*

Description

read in MSP file as list for ms/ms annotation

Usage

```
getms2pmd(file, digits = 2, icf = 10)
```

Arguments

file	the path to your MSP file
digits	mass or mass to charge ratio accuracy for pmd, default 2
icf	intensity cutoff, default 10 percentage

Value

list a list with MSP information for MS/MS annotation

getmspmd *read in MSP file as list for EI-MS annotation*

Description

read in MSP file as list for EI-MS annotation

Usage

```
getmspmd(file, digits = 2, icf = 10)
```

Arguments

file	the path to your MSP file
digits	mass or mass to charge ratio accuracy for pmd, default 0
icf	intensity cutoff, default 10 percentage

Value

list a list with MSP information for EI-MS annotation

getpaired *Filter ions/peaks based on retention time hierarchical clustering, paired mass distances(PMD) and PMD frequency analysis.*

Description

Filter ions/peaks based on retention time hierarchical clustering, paired mass distances(PMD) and PMD frequency analysis.

Usage

```
getpaired(
  list,
  rtcutoff = 10,
  ng = NULL,
  digits = 2,
  accuracy = 4,
  mdrange = NULL
)
```

Arguments

list	a list with mzrt profile
rtcutoff	cutoff of the distances in retention time hierarchical clustering analysis, default 10
ng	cutoff of global PMD's retention time group numbers, If ng = NULL, 20 percent of RT cluster will be used as ng, default NULL.
digits	mass or mass to charge ratio accuracy for pmd, default 2
accuracy	measured mass or mass to charge ratio in digits, default 4
mdrange	mass defect range to ignore. Default NULL and c(0.25,0.9) to retain the possible reaction related paired mass

Value

list with tentative isotope, multi-chargers, adducts, and neutral loss peaks' index, retention time clusters.

See Also

getstd,getsda,plotpaired

Examples

```
data(spmeinvivo)
pmd <- getpaired(spmeinvivo)
```

getpmd *Get pmd for specific reaction*

Description

Get pmd for specific reaction

Usage

```
getpmd(list, pmd, rtcutoff = 10, corcutoff = NULL, digits = 2, accuracy = 4)
```

Arguments

list	a list with mzrt profile
pmd	a specific paired mass distance or a vector of pmds
rtcutoff	cutoff of the distances in retention time hierarchical clustering analysis, default 10
corcutoff	cutoff of the correlation coefficient, default NULL
digits	mass or mass to charge ratio accuracy for pmd, default 2
accuracy	measured mass or mass to charge ratio in digits, default 4

Value

list with paired peaks for specific pmd or pmds.

See Also

getpaired,getstd,getsda,getrda

Examples

```
data(spmeinvivo)
pmd <- getpmd(spmeinvivo,pmd=15.99)
```

getpmddf *Get pmd details for specific reaction after the removal of isotopouge.*

Description

Get pmd details for specific reaction after the removal of isotopouge.

Usage

```
getpmddf(mz, group = NULL, pmd = NULL, digits = 2, mdrange = c(0.25, 0.9))
```

Arguments

mz	a vector of mass to charge ratio.
group	mass to charge ratio group from either retention time or mass spectrometry imaging segmentation.
pmd	a specific paired mass distance or a vector of pmds
digits	mass or mass to charge ratio accuracy for pmd, default 2.
mdrange	mass defect range to ignore. Default c(0.25,0.9) to retain the possible reaction related paired mass.

Value

dataframe with paired peaks for specific pmd or pmds. When group is provided, a column named net will be generated to show if certain pmd will be local(within the same group) or global(across the groups)

See Also

getpaired,getstd,getsda,getrda

Examples

```
data(spmeinvivo)
pmddf <- getpmddf(spmeinvivo$mz,pmd=15.99)
```

---

getposneg *Link pos mode peak list with neg mode peak list by pmd.*

Description

Link pos mode peak list with neg mode peak list by pmd.

Usage

```
getposneg(pos, neg, pmd = 2.02, digits = 2)
```

Arguments

pos	a list with mzrt profile collected from positive mode.
neg	a list with mzrt profile collected from negative mode.
pmd	numeric or numeric vector
digits	mass or mass to charge ratio accuracy for pmd, default 2

Value

dataframe with filtered positive and negative peak list

getrda *Perform structure/reaction directed analysis for mass only.*

Description

Perform structure/reaction directed analysis for mass only.

Usage

```
getrda(
  mz,
  pmd = NULL,
  freqcutoff = 10,
  digits = 3,
  top = 20,
  formula = NULL,
  mdrange = c(0.25, 0.9),
  verbose = FALSE
)
```

Arguments

mz	numeric vector for independent mass or mass to charge ratio. Mass to charge ratio from GlobalStd algorithm is suggested. Isomers would be excluded automated
pmd	a specific paired mass distance or a vector of pmds, default NULL
freqcutoff	pmd frequency cutoff for structures or reactions, default 10
digits	mass or mass to charge ratio accuracy for pmd, default 3
top	top n pmd frequency cutoff when the freqcutoff is too small for large data set
formula	vector for formula when you don't have mass or mass to charge ratio data
mdrange	mass defect range to ignore. Default c(0.25,0.9) to retain the possible reaction related paired mass
verbose	logic, if TURE, return will be llist with paired mass distances table. Default FALSE.

Value

logical matrix with row as the same order of mz or formula and column as high frequency pmd group when verbose is FALSE

See Also

getsda

Examples

```
data(spmeinvivo)
pmd <- getpaired(spmeinvivo)
std <- getstd(pmd)
sda <- getrda(spmeinvivo$mz[std$stdmassindex])
sda <- getrda(spmeinvivo$mz, pmd = c(2.016,15.995,18.011,14.016))
```

`getreact` *Get quantitative paired peaks list for specific reaction/pmd*

Description

Get quantitative paired peaks list for specific reaction/pmd

Usage

```
getreact(
  list,
  pmd,
  rtcutoff = 10,
  digits = 2,
  accuracy = 4,
  cvcutoff = 30,
  outlier = FALSE,
  method = "static",
  ...
)
```

Arguments

`list`	a list with mzrt profile and data
`pmd`	a specific paired mass distances
`rtcutoff`	cutoff of the distances in retention time hierarchical clustering analysis, default 10
`digits`	mass or mass to charge ratio accuracy for pmd, default 2
`accuracy`	measured mass or mass to charge ratio in digits, default 4
`cvcutoff`	ratio or intensity cv cutoff for quantitative paired peaks, default 30
`outlier`	logical, if true, outlier of ratio will be removed, default False.
`method`	quantification method can be 'static' or 'dynamic'. See details.
`...`	other parameters for getpmd

Details

PMD based reaction quantification methods have two options: 'static' will only consider the stable mass pairs across samples and such reactions will be limited by the enzyme or other factors than substrates. 'dynamic' will consider the unstable paired masses by normalization the relatively unstable peak with stable peak between paired masses and such reactions will be limited by one or both peaks in the paired masses.

Value

list with quantitative paired peaks.

See Also

getpaired,getstd,getsda,getrda,getpmd,

Examples

```
data(spmeinvivo)
pmd <- getreact(spmeinvivo,pmd=15.99)
```

---

getsda *Perform structure/reaction directed analysis for peaks list.*

Description

Perform structure/reaction directed analysis for peaks list.

Usage

```
getsda(
  list,
  rtcutoff = 10,
  corcutoff = NULL,
  digits = 2,
  accuracy = 4,
  freqcutoff = NULL
)
```

Arguments

list	a list with mzrt profile
rtcutoff	cutoff of the distances in retention time hierarchical clustering analysis, default 10
corcutoff	cutoff of the correlation coefficient, default NULL
digits	mass or mass to charge ratio accuracy for pmd, default 2
accuracy	measured mass or mass to charge ratio in digits, default 4
freqcutoff	pmd frequency cutoff for structures or reactions, default NULL. This cutoff will be found by PMD network analysis when it is NULL.

Value

list with tentative isotope, adducts, and neutral loss peaks' index, retention time clusters.

See Also

getpaired,getstd,plotpaired

Examples

```
data(spmeinvivo)
pmd <- getpaired(spmeinvivo)
std <- getstd(pmd)
sda <- getsda(std)
```

`getstd` *Find the independent ions for each retention time hierarchical clustering based on PMD relationship within each retention time cluster and isotope and return the index of the std data for each retention time cluster.*

Description

Find the independent ions for each retention time hierarchical clustering based on PMD relationship within each retention time cluster and isotope and return the index of the std data for each retention time cluster.

Usage

```
getstd(list, corcutoff = NULL, digits = 2, accuracy = 4)
```

Arguments

`list`	a list from getpaired function
`corcutoff`	cutoff of the correlation coefficient, default NULL
`digits`	mass or mass to charge ratio accuracy for pmd, default 2
`accuracy`	measured mass or mass to charge ratio in digits, default 4

Value

list with std mass index

See Also

getpaired,getsda,plotstd

Examples

```
data(spmeinvivo)
pmd <- getpaired(spmeinvivo)
std <- getstd(pmd)
```

`gettarget` *Get multiple injections index for selected retention time*

Description

Get multiple injections index for selected retention time

Usage

```
gettarget(rt, drt = 10, n = 6)
```

Arguments

`rt`	retention time vector for peaks in seconds
`drt`	retention time drift for targeted analysis in seconds, default 10.
`n`	max ions numbers within retention time drift windows

Value

index for each injection

Examples

```
data(spmeinvivo)
pmd <- getpaired(spmeinvivo)
std <- getstd(pmd)
index <- gettarget(std$rt[std$stdmassindex])
table(index)
```

`globalstd` *GlobalStd algorithm with structure/reaction directed analysis*

Description

GlobalStd algorithm with structure/reaction directed analysis

Usage

```
globalstd(
  list,
  rtcutoff = 10,
  ng = NULL,
  corcutoff = NULL,
  digits = 2,
  accuracy = 4,
  freqcutoff = NULL,
  mdrange = NULL,
  sda = FALSE
)
```

Arguments

list	a peaks list with mass to charge, retention time and intensity data
rtcutoff	cutoff of the distances in cluster, default 10
ng	cutoff of global PMD's retention time group numbers, If ng = NULL, 20 percent of RT cluster will be used as ng, default NULL.
corcutoff	cutoff of the correlation coefficient, default NULL
digits	mass or mass to charge ratio accuracy for pmd, default 2
accuracy	measured mass or mass to charge ratio in digits, default 4
freqcutoff	pmd frequency cutoff for structures or reactions, default NULL. This cutoff will be found by PMD network analysis when it is NULL.
mdrange	mass defect range to ignore. Default NULL and c(0.25,0.9) to retain the possible reaction related paired mass
sda	logical, option to perform structure/reaction directed analysis, default FALSE.

Value

list with GlobalStd algorithm processed data.

See Also

getpaired,getstd,getsda,plotstd,plotstdsda,plotstdrt

Examples

```
data(spmeinvivo)
re <- globalstd(spmeinvivo)
```

hmdb *A dataframe containing HMDB with unique accurate mass pmd with three digits frequency larger than 1 and accuracy percentage larger than 0.9.*

Description

A dataframe containing HMDB with unique accurate mass pmd with three digits frequency larger than 1 and accuracy percentage larger than 0.9.

Usage

```
data(hmdb)
```

Format

A dataframe with atoms numbers of C, H, O, N, P, S

percentage accuracy of atom numbers prediction

pmd2 pmd with two digits

pmd pmd with three digits

keggrall *A dataframe containing reaction related accurate mass pmd and related reaction formula with KEGG ID*

Description

A dataframe containing reaction related accurate mass pmd and related reaction formula with KEGG ID

Usage

```
data(keggrall)
```

Format

A dataframe with KEGG reaction, their realted pmd and atoms numbers of C, H, O, N, P, S

ID KEGG reaction ID

pmd pmd with three digits

MaConDa *mass spectrometry contaminants database for PMD check*

Description

mass spectrometry contaminants database for PMD check

Usage

```
data(MaConDa)
```

Format

A data frame from doi:10.1093/bioinformatics/bts527 with 308 rows and 5 variables:

id MaConDa ID

name contaminants

formula contaminants fomula

exact_mass exact mass of contaminants

type_of_contaminant type of contaminant

omics *A dataframe containing multiple reaction database ID and their related accurate mass pmd and related reactions*

Description

A dataframe containing multiple reaction database ID and their related accurate mass pmd and related reactions

Usage

```
data(omics)
```

Format

A dataframe with reaction and their realted pmd

KEGG KEGG reaction ID

RHEA_ID RHEA_ID

DIRECTION reaction direction

MASTER_ID master reaction RHEA ID

ec ec reaction ID

ecocyc ecocyc reaction ID

macie macie reaction ID

metacyc metacyc reaction ID

reactome reactome reaction ID

compounds reaction related compounds

pmd pmd with two digits

pmd2 pmd with three digits

`pcasf` *Compare matrices using PCA similarity factor*

Description

Compare matrices using PCA similarity factor

Usage

```
pcasf(x, y, dim = NULL)
```

Arguments

`x`	Matrix with sample in column and features in row
`y`	Matrix is compared to `x`.
`dim`	number of retained dimensions in the comparison. Defaults to all.

Value

Ratio of projected variance to total variance

Author(s)

Edgar Zanella Alvarenga

References

Singhal, A. and Seborg, D. E. (2005), Clustering multivariate time-series data. J. Chemometrics, 19: 427-438. doi: 10.1002/cem.945

Examples

```
c1 <- matrix(rnorm(16),nrow=4)
c2 <- matrix(rnorm(16),nrow=4)
pcasf(c1, c2)
```

plotcn *plot PMD KEGG network for certain compounds and output network average distance and degree*

Description

plot PMD KEGG network for certain compounds and output network average distance and degree

Usage

```
plotcn(formula, name, pmd)
```

Arguments

formula	Chemical formula
name	Compound name
pmd	specific paired mass distances

Examples

```
plotcn('C6H12O6','Glucose',c(2.016,14.016,15.995))
```

plotpaired *Plot the mass pairs and high frequency mass distances*

Description

Plot the mass pairs and high frequency mass distances

Usage

```
plotpaired(list, index = NULL, ...)
```

Arguments

list	a list from getpaired function
index	index for PMD value
...	other parameters for plot function

See Also

getpaired, globalstd

Examples

```
data(spmeinvivo)
pmd <- getpaired(spmeinvivo)
plotpaired(pmd)
```

plotrtg *Plot the retention time group*

Description

Plot the retention time group

Usage

```
plotrtg(list, ...)
```

Arguments

list	a list from getpaired function
...	other parameters for plot function

See Also

getpaired, globalstd

Examples

```
data(spmeinvivo)
pmd <- getpaired(spmeinvivo)
plotrtg(pmd)
```

plotsda *Plot the specific structure directed analysis(SDA) groups*

Description

Plot the specific structure directed analysis(SDA) groups

Usage

```
plotsda(list, ...)
```

Arguments

list	a list from getpmd function
...	other parameters for plot function

See Also

getstd, globalstd,plotstd,plotpaired,plotstdrt

Examples

```
data(spmeinvivo)
re <- getpmd(spmeinvivo,pmd=78.9)
plotsda(re)
```

`plotstd` *Plot the std mass from GlobalStd algorithm*

Description

Plot the std mass from GlobalStd algorithm

Usage

```
plotstd(list)
```

Arguments

`list`	a list from getstd function

See Also

`getstd`, `globalstd`

Examples

```
data(spmeinvivo)
pmd <- getpaired(spmeinvivo)
std <- getstd(pmd)
plotstd(std)
```

`plotstdrt` *Plot the std mass from GlobalStd algorithm in certain retention time groups*

Description

Plot the std mass from GlobalStd algorithm in certain retention time groups

Usage

```
plotstdrt(list, rtcluster, ...)
```

Arguments

list	a list from getstd function
rtcluster	retention time group index
...	other parameters for plot function

See Also

getstd, globalstd,plotstd,plotpaired,plotstdsda

Examples

```
data(spmeinvivo)
pmd <- getpaired(spmeinvivo)
std <- getstd(pmd)
plotstdrt(std,rtcluster = 6)
```

---

plotstdsda *Plot the std mass from GlobalStd algorithm in structure directed analysis(SDA) groups*

Description

Plot the std mass from GlobalStd algorithm in structure directed analysis(SDA) groups

Usage

```
plotstdsda(list, index = NULL, ...)
```

Arguments

list	a list from getsda function
index	index for PMD value
...	other parameters for plot function

See Also

getstd, globalstd,plotstd,plotpaired,plotstdrt

Examples

```
data(spmeinvivo)
re <- globalstd(spmeinvivo, sda=TRUE)
plotstdsda(re)
```

runPMD *Shiny application for PMD analysis*

Description

Shiny application for PMD analysis

Usage

```
runPMD()
```

runPMDnet *Shiny application for PMD network analysis*

Description

Shiny application for PMD network analysis

Usage

```
runPMDnet()
```

sda *A dataset containing common Paired mass distances of substructure, ions replacements, and reaction*

Description

A dataset containing common Paired mass distances of substructure, ions replacements, and reaction

Usage

```
data(sda)
```

Format

A data frame with 94 rows and 4 variables:

PMD Paired mass distances

origin potential sources

Ref. references

mode positive, negative or both mode to find corresponding PMDs

`spmeinvivo` *A peaks list dataset containing 9 samples from 3 fish with triplicates samples for each fish from LC-MS.*

Description

A peaks list dataset containing 9 samples from 3 fish with triplicates samples for each fish from LC-MS.

Usage

```
data(spmeinvivo)
```

Format

A list with 4 variables from 1459 LC-MS peaks:

mz mass to charge ratios

rt retention time

data intensity matrix

group group information

Index