Package 'pmd'

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Type Package

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

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Description Paired mass distance (PMD) analysis proposed in Yu, Olkowicz and Pawliszyn (2018) <doi:10.1016/j.aca.2018.10.062> 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. A GUI for PMD analysis is also included as a 'shiny' application.

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

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

License GPL-2

Encoding UTF-8

LazyData true

Suggests knitr, enviGCMS

VignetteBuilder knitr

biocViews

Depends R (>= 2.10)

Imports RColorBrewer, shiny, rmarkdown

RoxygenNote 6.1.0

NeedsCompilation no

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`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 = 10)
```

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

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)
```

---

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

Description

Perform structure/reaction directed analysis for peaks list.

Usage

```
getsda(list, rtcutoff = 10, freqcutoff = 10, corcutoff = NULL)
```

Arguments

list	a list with mzrt profile
rtcutoff	cutoff of the distances in retention time hierarchical clustering analysis, default 10
freqcutoff	cutoff of frequency of PMDs between RT cluster for peaks, default 10
corcutoff	cutoff of the correlation coefficient, default 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)
```

Arguments

list	a list from getpaired function
corcutoff	cutoff of the correlation coefficient, default NULL

Value

list with std mass index

See Also

getpaired,getsda,plotstd

Examples

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

globalstd *GlobalStd algorithm with structure/reaction directed analysis*

Description

GlobalStd algorithm with structure/reaction directed analysis

Usage

```
globalstd(list, rtcutoff = 10, ng = 10, corcutoff = NULL,
  freqcutoff = 10)
```

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
corcutoff	cutoff of the correlation coefficient, default NULL
freqcutoff	cutoff of frequency of PMDs between RT cluster for independent peaks, default 10

Value

list with GlobalStd algorithm processed data.

See Also

getpaired,getstd,getsda,plotstd,plotstdsda,plotstdrt

Examples

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

---

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)
```

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)
plotstdsda(re)
```

runPMD *Shiny application for PMD analysis*

Description

Shiny application for PMD analysis

Usage

```
runPMD()
```

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 potentical 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

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