Package 'Miso'

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Type Package

Title Multi-Isotope Labeling for Metabolomics Analysis

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Author Yonghui Dong

Maintainer Yonghui Dong <yonghui.dong@gmail.com>

Description An efficient approach for fishing out the dual (or multiple) isotope labeled analytes using dual labeling of metabolites for metabolome analysis (DLEMMA) approach, described in Liron (2018) <doi:10.1021/acs.analchem.8b01644>.

Depends R (>= 2.10),

Imports S4Vectors, stats, utils, dplyr, plotly

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NeedsCompilation no

Repository CRAN

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R topics documented:

diso *Isotope filtering*

Description

filtering isotopically labeled analytes according to RT and mass differences

Usage

```
diso(iso1, n11, n12, iso2 = "NO", n21 = 0, n22 = 0, exp.base,
  exp.iso, ppm = 10, rt.dif = 6)
```

Arguments

iso1	the first labled atom in precusor ion.
n11	the maximum numbers of the first labled atoms expected in the labeled intermediates.
n12	the minimum numbers of the first labled atoms expected in the labeled intermediates.
iso2	the second labled atom in the same precusor ion, default value 'NO' (not exist).
n21	the maximum numbers of the second labled atoms expected in the labeled intermediates, default value 0.
n22	the minimum numbers of the second labled atoms expected in the labeled intermediates, default value 0.
exp.base	the control group (fed with unlabled precusor).
exp.iso	isotope labeled group.
ppm	m/z tolarance, default value 30.
rt.dif	retention time tolarance, default value 6 seconds.

Value

results containing unlabled and their corresponding labled analytes, with RT and labeling information.

Examples

```
data(lcms)
explist <- prefilter(lcms[1: 100, ]) # use a subset of lcms data as example
exp.B <- explist$exp.B
exp.C <- explist$exp.C
exp.D <- explist$exp.D
iso.C <- diso(iso1 = 'H2', n11 = 4, n12 = 2, exp.base = exp.B, exp.iso = exp.C)
iso.D <- diso(iso1 = 'C13', n11 = 9, n12 = 6, iso2 = 'N15', n21 = 1, n22 = 0,
exp.base = iso.C[,1:3], exp.iso = exp.D)
```

fold *fold change*

Description

calculate fold change among different samples.

Usage

```
fold(x, f)
```

Arguments

x	matrix data, type: matrix
f	groups

Value

a dataframe with fold changes

Examples

```
vars <- 1000
samples <- 50
groups <- 3
dat <- replicate(vars, runif(n = samples))
f <- rep_len(1:groups, samples) + 1
f <- LETTERS[f]
ret <- fold(dat, f)
```

Fresult *Full result list*

Description

export full isotope labeled result list

Usage

```
Fresult(iso.C, iso.D)
```

Arguments

iso.C	result from the first labeled precusor from Exp. C
iso.D	result from the second labled precusor from Exp. D

Value

file containing the all the possible combined results. Full list, but redundant

Examples

```
data(lcms)
explist <- prefilter(lcms[1: 100, ]) # use a subset of lcms data as example
exp.B <- explist$exp.B
exp.C <- explist$exp.C
exp.D <- explist$exp.D
iso.C <- diso(iso1 = 'H2', n11 = 4, n12 = 3, exp.base = exp.B, exp.iso = exp.C)
iso.D <- diso(iso1 = 'C13', n11 = 9, n12 = 6, iso2 = 'N15', n21 = 1, n22 = 0,
exp.base = iso.C[,1:3], exp.iso = exp.D)
full_Result <- Fresult(iso.C, iso.D)
```

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getp *get p-values*

Description

get p-values from Post Hoc analysis

Usage

```
getp(dat)
```

Arguments

dat	peaklist

Value

a data frame

Examples

```
dat = as.data.frame(matrix(runif(2*300), ncol = 2, nrow = 300))
dat$group = rep(LETTERS[2:4], 100)
out <- getp(dat)
```

isoplot *plot isotopologues*

Description

plot unlabled and labeled Isotopologues from filtering result

Usage

```
isoplot(dat, rinx)
```

Arguments

dat	isotope filtering result
rinx	row index

Value

interactive plot

Examples

```
data(lcms)
explist <- prefilter(lcms[1: 500, ]) # use a subset of lcms data as example
exp.B <- explist$exp.B
exp.C <- explist$exp.C
exp.D <- explist$exp.D
iso.C <- diso(iso1 = 'H2', n11 = 4, n12 = 3, exp.base = exp.B, exp.iso = exp.C)
iso.D <- diso(iso1 = 'C13', n11 = 9, n12 = 6, iso2 = 'N15', n21 = 1, n22 = 0,
exp.base = iso.C[,1:3], exp.iso = exp.D)
full_Result <- Fresult(iso.C, iso.D)
reduced_Result <- Rresult(full_Result)
isoplot(full_Result, 1)
```

lcms *LC-MS peaklist*

Description

A LC-MS dataset containing the analytes from 5 experimental groups lcms. The variables are as follows:

Usage

```
data(lcms)
```

Format

A data frame with 16133 rows and 22 variables

Details

- mz.
- mzmin.
- mzmax.
- rt.
- rtmin.
- rtmax.
- npeaks.
- A.
- B.
- C.
- D.
- E.
- X11Feb15_04n.
- X11Feb15_05n.
- X11Feb15_06n.
- X11Feb15_07n.
- X11Feb15_08n.
- X11Feb15_09n.
- X11Feb15_11n.
- X11Feb15_12n.
- X11Feb15_13n.
- X11Feb15_14n.

Examples

```
data(lcms)
```

prefilter *Prefilter*

Description

prefiltering isotopically labeled analytes according to the experiment design.

Usage

```
prefilter(peak, cutint = 0, nsam = 2, minsam = 1)
```

Arguments

peak	xcms processed dataset.
cutint	cutoff intensity. Ion intensity below the cutoff value will be considered as noise, default value 0.
nsam	number of samples in each experiment, default value 2. If the sample numbers are different in each gorup, a vector can be used to input the number of samples in each group, i.e. nsam = c(0, 2, 2, 3, 3).
minsam	minimum number of samples.The peak is considered valid only when it is at least detected in the minimum number of samples in a group, default value 1. A vector can be used to To control the minsam in each group, i.e. nsam = c(1, 1, 2, 2, 1).

Value

a filtered peaklist.

Examples

```
data(lcms)
explist <- prefilter(lcms[1:100, ])
```

prefilter2 *Prefilter2*

Description

prefiltering isotopically labeled analytes according to the experiment design.

Usage

```
prefilter2(peak, nsam = 2, p = 0.05, fold = 10)
```

Arguments

peak	xcms processed dataset.
nsam	number of samples in each experiment, default value = 2. If the sample numbers are different in each gorup, a vector can be used to input the number of samples in each group, i.e. nsam = c(0, 2, 2, 3, 3).
p	p-value threshold, default value = 0.05
fold	fold change threshold, default value = 10

Value

a filtered peaklist

Examples

```
data(lcms)
explist <- prefilter2(lcms[1:100, ])
```

Rresult *Reduced result list*

Description

export reduced isotope labeled result list

Usage

```
Rresult(full_Result, cutint = 0)
```

Arguments

full_Result	full result list
cutint	cutoff intensity.Rows that any ion intensities below the cutoff value will removed

Value

csv file with repeated results being removed

Examples

```
data(lcms)
explist <- prefilter(lcms[1: 100, ]) # use a subset of lcms data as example
exp.B <- explist$exp.B
exp.C <- explist$exp.C
exp.D <- explist$exp.D
iso.C <- diso(iso1 = 'H2', n11 = 4, n12 = 3, exp.base = exp.B, exp.iso = exp.C)
iso.D <- diso(iso1 = 'C13', n11 = 9, n12 = 6, iso2 = 'N15', n21 = 1, n22 = 0,
```

```
exp.base = iso.C[,1:3], exp.iso = exp.D)
full_Result <- Fresult(iso.C, iso.D)
reduced_Result <- Rresult(full_Result)
```

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