

Package ‘mQTL’

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Description mQTL provides a complete QTL analysis pipeline for metabolomic data. Distinctive features include normalisation using PQN approach, peak alignment using RSPA approach, dimensionality reduction using SRV approach and finally QTL mapping using R/qlt package.

License GPL

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mQTL-package

Metabolomic Quantitative Trait Locus mapping

Description

mQTL provides a complete QTL analysis pipeline for 1H NMR data. Distinctive features include normalisation using QPN approach, peak alignment using RSPA approach, dimensionality reduction using SRV approach and finally QTL mapping using R/qlt package.

Details

Package: mQTL
Type: Package
Version: 1.0
Date: 2013-09-18
License: GPL (>= 3)

Main fuctions:

- format_mQTL: creates the proper format of data
- align_mQTL: peak alignment and normalisation
- pre_mQTL: dimension reduction by statistical recoupling of variables
- process_mQTL: computes LODs using extended Haley-Knott method
- post_mQTL: plots the results of a given run
- summary_mQTL: provides the results as a table

Author(s)

Lyamine Hedjazi and Jean-Baptiste Cazier

Maintainer: Lyamine Hedjazi <<1.hedjazi@fondation-ican.com>>

alignSp *Base function for Spectrum Alignment*

Description

Alignment of spectrum segment to a spectrum of interest

Usage

```
alignSp(refSp, refSegments, intSp, intSegments, recursion, MAX_DIST_FACTOR, MIN_RC)
```

Arguments

| | |
|-----------------|--|
| refSp | reference spectrum |
| refSegments | reference segments |
| intSp | spectrum of interest |
| intSegments | segments of interest |
| recursion | parameters for recursive alignment |
| MAX_DIST_FACTOR | the distance matching parameter (0.5*peak width) |
| MIN_RC | minimum resamblance coefficient |

Value

| | |
|------------------|-------------------|
| alignedSpectrum | aligned spectrum |
| extendedSegments | extended segments |

Author(s)

Lyamine Hedjazi

Maintainer: Lyamine Hedjazi <<l.hedjazi@fondation-ican.com>>

See Also

[align_mQTL](#)

Examples

```
## Not run:  
## Data  
  
Sp=matrix(rnorm(10*13454,mean=0,sd=1), nrow=10,ncol=13454)
```

```

##Segmentation parameters

peakParam=list()
peakParam$ppmDist <- 0.03 #(ppm) # distance to concatenate adjacent peaks #default 0.03#
peakParam$ampThr <- 0.3 # amplitude value to threshold small peaks
peakParam$minPeakWidth <- 0.005 # min peak width in ppm scale
peakParam$iFrameLen<-11 # Savitzky-Golay frame length in ppm scale
peakParam$iOrder<-3 # polynomial order of Savitzky - Golay filter
peakParam$peakEdgeMax<-0.2 # maximal peak edge

##Recursion alignment parameters

recursion=list()
recursion$resemblance<-0.95# Stop criterium of the recursion indicating
#the complete alignment of segment peaks
recursion$segShift<-0.02#(ppm) max peak shift for large peaks
recursion$inbetweenShift<-0.02 #(ppm) max shift for small peaks
recursion$acceptance<-0.5 # if resemblance after the alignment between modified test
recursion$minSegWidth<-0.01 #(ppm) Stop criteria of the recursion - the size of the smallest peak
recursion$step<-0.02 # Recursion step (default 0.02)

## Normalisation

normD<-normalise(Sp,'prob')

## Reference spectrum selection

index<-selectRefSp(normD$Sp,recursion$step)
refSp<-normD$Sp[index,] # reference spectrum picked-up

##segmentate a reference spectrum

refSegments<- segmentateSp(refSp, peakParam) # segmentate reference spectrum

##segmentate a test spectrum

spectrum<-normD$Sp[10,]
testSegments<- segmentateSp(spectrum, peakParam) # segmentate test spectrum (10th sample)

#match test and reference segments

attachedSegs<-attachSegments(refSegments,testSegments)

refSegments<-attachedSegs$refSegmentsNew
testSegments<-attachedSegs$testSegmentsNew

##matching parameters

MAX_DIST_FACTOR<-0.5 # The distance matching parameter (0.5*peak_width)
MIN_RC<-0.25 # Minimum resemblance coefficient

Segs<-matchSegments(refSp,spectrum, testSegments,refSegments,MAX_DIST_FACTOR,MIN_RC)

```

```
#align a test spectrum

refSgs<-Segs$refSegs
tstSgs<-Segs$testSegs

SpAlg<- alignSp(refSp,refSgs,spectrum,tstSgs,recursion,MAX_DIST_FACTOR,MIN_RC)

## End(Not run)
```

align_mQTL

Peak alignment and normalisation of metabolomic data

Description

Recursive Segment-Wise Peak Alignment (RSPA) for accounting peak position variation across metabolomic data

Usage

```
align_mQTL(datafile, outdat)
```

Arguments

| | |
|----------|-----------------|
| datafile | raw spectra |
| outdat | aligned spectra |

Details

The algorithm is based on the following workflow:

1. Quotient probabilistic normalisation of metabolomic data.
2. Automatic selection of a reference spectrum.
3. Segmentate a reference spectrum.
4. Then for each test spectrum:
 - segmentate a test spectrum.
 - match test and reference segments.
 - align a test spectrum.

Value

It returns aligned data.

Author(s)

Lyamine Hedjazi

References

Veselkov, K. et al (2009) Recursive Segment-Wise Peak Alignment of Biological ¹H NMR Spectra for Improved Metabolic Biomarker Recovery, *Anal. Chem.*, 81(1), 56-66.

See Also

[alignSp](#), [attachSegments](#), [matchSegments](#), [segmentateSp](#), [format_mQTL](#), [format_mQTL](#)

Examples

```
## Not run:
## Align metabolomic data profiles

cleandat<-"CleanMetaboFile.dat" ## Metabolomic data file in csvs format
aligdat<-"AlignData.dat" ## Aligned metabolomic profiles in csvs format

align_mQTL(cleandat,aligdat)

## End(Not run)
```

attachSegments

Concatenation of test and reference segments

Description

Concatenation of test and reference segments to ensure one-to-one correspondence.

Usage

```
attachSegments(refSegments, testSegments)
```

Arguments

| | |
|--------------|------------------------------------|
| refSegments | segments of the reference spectrum |
| testSegments | segments of the test spectrum |

Details

The algorithm:

1. For each reference segment within segment boundaries, i.e. between initial and final positions, find all centre (middle) positions of test segments and merge those segments, if more than one centre position is found
2. Apply the same procedure for each test segment

Value

A list:

segments\$start start of each concatenated test segment
 segments\$PeakLeftBoundary peak left boundary of each concatenated test segment
 segments\$PeakRightBoundary peak right boundary of each concatenated test segment
 segments\$Peaks peaks of each concatenated test segment
 segments\$end end of each concatenated test segment
 segments\$end center of each concatenated test segment

Author(s)

Lyamine Hedjazi

References

Veselkov, K. et al (2009) Recursive Segment-Wise Peak Alignment of Biological ¹H NMR Spectra for Improved Metabolic Biomarker Recovery, *Anal. Chem.*, 81(1), 56-66.

See Also

[matchSegments](#)

Examples

```
## Not run:

## Data

Sp=matrix(rnorm(10*13454,mean=0,sd=1), nrow=10,ncol=13454)

##Segmentation parameters

peakParam=list()
peakParam$ppmDist <- 0.03# (ppm) # distance to concatenate adjacent peaks #default 0.03#
peakParam$ampThr <- 0.3 # amplitude value to threshold small peaks #
peakParam$minPeakWidth <- 0.005 #min peak width in ppm scale
peakParam$iFrameLen<-11 #Savitzky-Golay frame length in ppm scale
peakParam$iOrder<-3 #polynomial order of Savitzky - Golay filter
peakParam$peakEdgeMax<-0.2

##Reference spectrum selection

step<-0.02 # Recursion step (default 0.02)
index<-selectRefSp(Sp,step)
refSp<-Sp[index,]
```

```
#segmentate a reference spectrum

refSegments<- segmentateSp(refSp, peakParam) # segmentate reference spectrum

#segmentate a test spectrum

spectrum<-Sp[10,]
testSegments<- segmentateSp(spectrum, peakParam) # segmentate test spectrum (10th sample)

# match test and reference segments

attachedSegs<-attachSegments(refSegments, testSegments)

## End(Not run)
```

format_mQTL

Routine to reformat the data into the required format

Description

This function enables to reformat data into the proper format. The user should provides in input metabolomic dataset, Genotype dataset and a dataset containing sex and pgm (parental grandmother).

Usage

```
format_mQTL(datafile, genofile, physdat, outdat, outgeno)
```

Arguments

| | |
|----------|--|
| datafile | metabolomic data file |
| genofile | genotype data file |
| physdat | a file containing sex and pgm |
| outdat | phenotype data (metabolomic data + sex + pgm) in the format csvs |
| outgeno | genotype data |

Value

It returns phynotype and genotype files in the proper format

Author(s)

Lyamine Hedjazi

See Also

[align_mQTL](#),

Examples

```

## Not run:
## Clean the raw data to match the genotype and phenotype and create the proper format

rawfile<-"MetaboFile.dat" ## Metabolomic data file
genofile<-"GenoFile.dat" ## Genotype data file
physiodat="physiodat.dat" ## data file containing sex and pgm
cleandat<-"CleanMetaboFile.dat" ## Metabolomic data file in csvs format
cleangen<-"CleanGenoFile.dat" ## Genotype data file in csvs format

format_mQTL(rawfile,genofile,physiodat, cleandat,cleangen)

## End(Not run)

```

matchSegments

Matching of the segment of interest to the corresponding reference

Description

The algorithm makes use of a fuzzy logic approach to match the segment of interest to the corresponding reference

Usage

```
matchSegments(refSp, intSp, intSegments, refSegments, MAX_DIST_FACTOR, MIN_RC)
```

Arguments

| | |
|-----------------|--|
| refSp | spectrum of reference |
| intSp | spetcrum of interest (test spectrum) |
| intSegments | segments of spectrum of interest |
| refSegments | segments of reference spectrum |
| MAX_DIST_FACTOR | the distance matching parameter (0.5*peak_width) |
| MIN_RC | minimum resamblance coefficient |

Details

Algorithm:

1. take segment of interest
2. take reference segments
3. calculate relative distance between them
4. calculate relative resamblance between them
5. find min value of relative distance and resamblance
6. use it as representative of similiarity between target and reference segments
7. find the segment that has the highest value of both relative distance and resamblance

Value

A list:

| | |
|----------|----------------------------|
| testSegs | matched test segments |
| refSegs | matched reference segments |

Author(s)

Lyamine Hedjazi

References

Veselkov, K. et al (2009) Recursive Segment-Wise Peak Alignment of Biological ¹H NMR Spectra for Improved Metabolic Biomarker Recovery, *Anal. Chem.*, 81(1), 56-66.

See Also

[attachSegments](#)

Examples

```
## Not run:

# Data

Sp=matrix(rnorm(10*13454,mean=0,sd=1), nrow=10,ncol=13454)

##Segmentation parameters

peakParam=list()
peakParam$ppmDist <- 0.03# (ppm) # distance to concatenate adjacent peaks #default 0.03#
peakParam$ampThr <- 0.3 # amplitude value to threshold small peaks #
peakParam$minPeakWidth <- 0.005 #min peak width in ppm scale
peakParam$iFrameLen<-11 #Savitzky-Golay frame length in ppm scale
peakParam$iOrder<-3 #polynomial order of Savitzky - Golay filter
peakParam$peakEdgeMax<-0.2

##reference spectrum selection

step=0.02 # Recursion step (default 0.02)
index<-selectRefSp(Sp,step)
refSp<-Sp[index,]

#segmentate a reference spectrum

refSegments<- segmentateSp(refSp, peakParam) # segmentate reference spectrum

#segmentate a test spectrum

spectrum<-Sp[10,]
```

```
testSegments<- segmentateSp(spectrum, peakParam) # segmentate test spectrum (10th sample)

#attach test and reference segments
attachedSegs<-attachSegments(refSegments, testSegments)

##Matching parameters

MAX_DIST_FACTOR<-0.5 # The distance matching parameter (0.5*peak_width)
MIN_RC<-0.25 # Minimum resamblance coefficient

refSegments<-attachedSegs$refSegmentsNew
testSegments<-attachedSegs$testSegmentsNew
Segs<-matchSegments(refSp, spectrum, testSegments, refSegments, MAX_DIST_FACTOR, MIN_RC)

## End(Not run)
```

normalise

Normalisation of metabolomic data

Description

Removing dilutions between biofluid samples (normalisation of spectra)

Usage

```
normalise(X, method)
```

Arguments

| | |
|--------|--|
| X | metabolomic data |
| method | total area (method<-"total") or quotient probabilistic method (method<-"prob") |

Value

normalised spectrum

Author(s)

Lyamine Hedjazi

References

Dieterle, F., et al (2006) Probabilistic Quotient Normalization as Robust Method to Account for Dilution of Complex Biological Mixtures. Application in 1H NMR Metabonomics, Anal. Chem., 78(13), 4281-4290.

See Also

[SRV](#)

Examples

```
## Data
Sp=matrix(rnorm(10*13454,mean=0,sd=1), nrow=10,ncol=13454)

## Quotient probabilistic normalisation
NormDat<-normalise(abs(Sp), 'prob')
```

| | |
|-----------|-------------------------------|
| peakPeaks | <i>Peak picking algorithm</i> |
|-----------|-------------------------------|

Description

Identification of peaks in metabolomic data based on the calculation of smoothed derivatives using Savitzky-Golay filter. The peak is identified if derivative crosses zero, i.e. $\text{sign}(X'(i)) > \text{sign}(X'(i+1))$.

Usage

```
peakPeaks(SpSmooth, dpDerivs, Sp)
```

Arguments

| | |
|----------|-------------------------------------|
| SpSmooth | smoothed spectrum |
| dpDerivs | smoothed derivative of the spectrum |
| Sp | Spectrum of interest |

Value

identified peaks

Author(s)

Lyamine Hedjazi

References

Veselkov, K. et al (2009) Recursive Segment-Wise Peak Alignment of Biological ¹H NMR Spectra for Improved Metabolic Biomarker Recovery, *Anal. Chem.*, 81(1), 56-66.

See Also

[sgolayDeriv](#)

Examples

```
## Data
Sp=matrix(rnorm(10*13454,mean=0,sd=1), nrow=10,ncol=13454)

## Peak picking
Spectrum<-Sp[1,]
iOrder <- 3
iFrameLen<- 11

SpDerivs=sgolayDeriv(Spectrum,iOrder,iFrameLen,2)
SpSmooth = sgolayDeriv(Spectrum,iOrder,iFrameLen,1)
peaks=peakPeaks(SpSmooth,SpDerivs,Spectrum)
```

post_mQTL

Plot top LOD results

Description

Function to plot the results of a given run

Usage

```
post_mQTL(results, probs = c(0.95, 0.99, 0.999, 0.9999))
```

Arguments

| | |
|---------|---|
| results | results of mQTL analysis. |
| probs | numeric vector of probabilities with values in [0,1]. (Values up to 2e-14 outside that range are accepted and moved to the nearby endpoint.). |

Details

This function plots different results corresponding to top LOD marker

Value

It returns graphs and summaries

Author(s)

Jean-Baptiste Cazier

See Also

[pre_mQTL](#)

Examples

```

## Not run:
## Pre-process data

infile<-"ReducedData.dat" ## Reduced data by SRV
cleangen<-"CleanGenoFile.dat" ## Genotype data file in csvs format
nperm <- 0 ## Number of permutations
MQTL_results<-process_mQTL(infile, cleangen, nperm)

post_mQTL(results)## Plot mQTL results

## End(Not run)

```

ppersp

Plot a 3-D profile of LODs

Description

Plot 3-D profile of LODs as function of genomic position and chemical shift

Usage

```
ppersp(z, ppm, titre, theta=-15, phi=15, r=50)
```

Arguments

| | |
|-------|---|
| z | table of results |
| ppm | chemical shift |
| titre | title |
| theta | angle defining the viewing direction (azimuthal direction) |
| phi | angle defining the viewing direction (colatitude direction) |
| r | the distance of the eyepoint from the centre of the plotting box. |

Value

plot 2D-profile

Author(s)

Jean-Baptiste Cazier

See Also

[pplot](#)

Examples

```
## Plot 3D profile

## Not run:
x11(width=5,height=5,pointsize=5)
titel<-"Example plot"
ppersp(results, ppm, title)

## End(Not run)
```

pplot

Plot a color scale layer

Description

Plot the results with a color scale y layer over 3 in 2D

Usage

```
pplot(z, titre, ppm, res, LT = c(5,10,15,20))
```

Arguments

| | |
|-------|---|
| z | mQTL's whole results |
| titre | figure title |
| ppm | chemical shift |
| res | results to be plotted |
| LT | quantil(res,probs), res: results and probs: vector of probabilities |

Value

2-D profile

Author(s)

Jean-Baptiste Cazier

See Also

[ppersp](#)

Examples

```
## Not run:  
  
## Plot 3D profile  
  
x11(width=5,height=5,pointsize=5)  
titel<-"Example plot"  
  
probs=c(0.95,0.99,0.999,0.9999) ## probabilities  
  
pplot(res,"Full 2D Profile", ppm, best, quantile(res,probs=probs))  
  
## End(Not run)
```

pre_mQTL

Statistical Recoupling of variables for mQTL analysis

Description

Makes use of SRV to preprocess metabolomic data for dimensionality reduction by statistical recoupling of variables

Usage

```
pre_mQTL(infile, outfile, met, corrT = 0.9)
```

Arguments

| | |
|---------|------------------------------|
| infile | metabolomic datafile |
| outfile | reduced metabolomic datafile |
| met | used statistical summary |
| corrT | correlation threshold |

Details

The SRV algorithm forms clusters of variables using a measure of a local spectral dependency. Then tests whether consecutive clusters are correlated to aggregate them into a single supercluster.

Value

The algorithm:

1. variables are associated into a series of clusters.
2. integration of clusters into superclusters.

Author(s)

Jean-Baptiste Cazier and Lyamine Hedjazi

References

Blaise,B. et al (2009) Statistical recoupling prior to significance testing in nuclear magnetic resonance based metabonomics, Anal. Chem., 81(15), 6242-6251.

See Also

[SRV,post_mQTL](#)

Examples

```
## Not run:
## Pre-process data

infile<-"AlignData.dat" ## Aligned metabolomic profiles in csvs format
outfile<-"ReducedData.dat" ## Reduced data by SRV
met<- "rectangle" ## Summary measure (mean, max,...)
corrT<- 0.9 ## Correlation threshold (default 0.9)
(pre_mQTL(infile, outfile, met, corrT)

## End(Not run)
```

process_mQTL

mQTL mapping

Description

Function to process the tissue extract of the individuals for QTL analysis

Usage

```
process_mQTL(datfile, genfile, nperm = 0)
```

Arguments

| | |
|---------|----------------|
| datfile | phenotype data |
| genfile | genotype data |
| nperm | nperm |

Details

This function makes use of metabolomic and genotype data to perform QTL analysis based on the R/QTL package, for mapping quantitative trait loci. In particular, it makes use of the extended Haley-Knott method to optimize the LOD score evaluation and avoid problems with missing genotypes.

Value

2D LOD score table

Author(s)

Jean-Baptiste Cazier and Hedjazi Lyamine

References

Broman, K., et al (2006) R/qtl: QTL mapping in experimental crosses, *Bioinformatics*, 19(7), 889-890.

See Also

[post_mQTL](#)

Examples

```
## Not run:
## Pre-process data
infile<-"ReducedData.dat" ## Reduced data by SRV
cleangen<-"CleanGenoFile.dat" ## Genotype data file in csvs format
nperm <- 0 ## Number of permutations
MQTL_results<-process_mQTL(infile, cleangen, nperm)

## End(Not run)
```

segmentateSp

Segmentation of a spectrum of interest

Description

Determination of highly intensive peaks in the spectrum of interest and subsequent concatenation of closely located peaks into larger segments

Usage

```
segmentateSp(Sp, peakParam)
```

Arguments

| | |
|-----------|---|
| Sp | spectrum |
| peakParam | a list: <ul style="list-style-type: none"> • ampThr: amplitude threshold [default 2*median(peaksMaxValues)] • iFrameLen: Savitzky-Golay frame length • iOrder: polynomial order of Savitzky - Golay filter • iFrameLen: Savitzky-Golay frame length • minPeakWidth: min peak size • ppmDist: distance to concatenate adjacent peaks |

Value

A list:

```
testSegmentsNew
                new test segments
refSegmentsNew new reference segments
```

Author(s)

Lyamine Hedjazi

References

Veselkov, K. et al (2009) Recursive Segment-Wise Peak Alignment of Biological ¹H NMR Spectra for Improved Metabolic Biomarker Recovery, *Anal. Chem.*, 81(1), 56-66.

See Also

[attachSegments](#), [matchSegments](#)

Examples

```
# Data

Sp=matrix(rnorm(10*13454,mean=0,sd=1), nrow=10,ncol=13454)

##Segmentation parameters

peakParam=list()
peakParam$ppmDist <- 0.03# (ppm) # distance to concatenate adjacent peaks #default 0.03#
peakParam$ampThr <- 0.3 # amplitude value to threshold small peaks #
peakParam$minPeakWidth <- 0.005 #min peak width in ppm scale
peakParam$iFrameLen<-11 #Savitzky-Golay frame length in ppm scale
peakParam$iOrder<-3 #polynomial order of Savitzky - Golay filter
peakParam$peakEdgeMax<-0.2

#segmentate a test spectrum (10th sample)

Spectr<-Sp[10,]
testSegments<- segmentateSp(Spectr, peakParam)
```

selectRefSp

Automated selection of a reference spectrum

Description

The selection of reference spectrum among all spectrums is based on the highest similarity to all other spectra

Usage

```
selectRefSp(X, step)
```

Arguments

| | |
|------|--|
| X | spectra |
| step | used to scale spectral regions down to specific bin size |

Value

returns the index of selected spectrum

Author(s)

Lyamine Hedjazi

See Also

[alignSp](#)

Examples

```
# Data
Sp=matrix(rnorm(10*13454,mean=0,sd=1), nrow=10,ncol=13454)

# Reference spectrum selection

step=0.02 # Recursion step (default 0.02)
index<-selectRefSp(Sp,step)
```

sgolay

Find the matrix of differentiation filters

Description

designs a Savitzky-Golay (polynomial) FIR smoothing filter. The polynomial order must be less than the frame size which must be odd.

Usage

```
sgolay(k,F,W)
```

Arguments

| | |
|---|------------------|
| k | polynomial order |
| F | frame size |
| W | weighting matrix |

Value

matrix of differentiators

Author(s)

Lyamine Hedjazi

References

Sophocles J. Orfanidis, INTRODUCTION TO SIGNAL PROCESSING, Prentice-Hall, 1995, Chapter 8

See Also

[sgolayDeriv](#)

Examples

```
k <- 3
F <- 11

Sg=sgolay(k,F)
```

sgolayDeriv

Calculate smoothed derivatives

Description

Calculate smoothed derivatives using Savitzky-Golay filter

Usage

```
sgolayDeriv(dpSpectr, iOrder, iFrameLen, j)
```

Arguments

| | |
|-----------|---|
| dpSpectr | input spectrum |
| iOrder | polynomial order of Savitzky - Golay filter |
| iFrameLen | Savitzky-Golay frame length in ppm scale |
| j | order of derivative |

Value

jth dervitative of the spectrum

Author(s)

Lyamine Hedjazi

See Also

[sgolay](#)

Examples

```
## Data

Sp=matrix(rnorm(10*13454,mean=0,sd=1), nrow=10,ncol=13454)

## Peak picking
Spectrum<-Sp[10,]
iOrder <- 3
iFrameLen<- 11
j<-2

SpDerivs=sgolayDeriv(Spectrum,iOrder,iFrameLen,j)
```

SRV

Statistical Recoupling of Variables

Description

Base function for dimensionality reduction by statistical recoupling of variables

Usage

```
SRV(X, minsize, correl, clustf = median)
```

Arguments

| | |
|---------|-----------------------|
| X | data matrix |
| minsize | singlet size |
| correl | bucketting resolution |
| clustf | correlation threshold |

Value

A list:

indicesdebf starting border of superclusters
indicesfinf ending border of superclusters

Author(s)

Jean-Baptiste Cazier

References

Blaise,B. et al (2009) Statistical recoupling prior to significance testing in nuclear magnetic resonance based metabonomics, Anal. Chem., 81(15), 6242-6251.

See Also

[pre_mQTL](#)

Examples

```
## Not run:  
  
## Statistical recoupling of variables  
  
    corrT=0.9 # correlation threshold  
    minsize=10 # singlet size  
    met="rectangle" # summary measure  
  
#Perform the SRV analysis to reduce the number of dimension of Spectra data (Sp)  
  
    SRV<-SRV(Sp, minsize, corrT,clustf=met)  
  
## End(Not run)
```

SRV_Corr

Statistical recoupling of variables in a supervised context

Description

Correlation generation for Statistical Recoupling of Variables.

Usage

```
SRV_Corr(X, Y, minsize, correl)
```

Arguments

| | |
|---------|-----------------------|
| X | data matrix |
| Y | class matrix |
| minsize | bucketting resolution |
| correl | correlation threshold |

Value

A list:

| | |
|--------------|---------------------------------------|
| Pfinal | pvalue vector |
| indicesdebf | starting border of cluster |
| indicesfinfl | ending border of cluster |
| Correlation | Correlation of superclusters/clusters |

Author(s)

Jean-Baptiste Cazier

References

Blaise,B. et al (2009) Statistical recoupling prior to significance testing in nuclear magnetic resonance based metabonomics, Anal. Chem., 81(15), 6242-6251.

See Also

[SRV](#), [pre_mQTL](#)

summary_mQTL

Function to summarize the results of a all the runs and their differences

Description

This function generates a table containing the genetic markers and thier associated metabolomic variables and estimated LOD score.

Usage

```
summary_mQTL(results, Th = 5)
```

Arguments

| | |
|---------|-----------------------------------|
| results | mQTL mapping results |
| Th | Threshold of the top accepted LOD |

Details

Generates a text file containing a table of results

Value

returns Summaries

Author(s)

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See Also

[pre_mQTL](#)

Examples

```
## Not run:

## Pre-process data

infile<-"ReducedData.dat" ## Reduced data by SRV
cleangen<-"CleanGenoFile.dat" ## Genotype data file in csvs format
nperm <- 0 ## Number of permutations
MQTL_results<-process_mQTL(infile, cleangen, nperm)

T=10 ## LOD threshold
summary_mQTL(results,T=8)## summarizes mQTL results in a table

## End(Not run)
```

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