Package 'speaq'

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Type Package

Title An R-package for NMR spectrum alignment and quantitation

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Description Integrated NMR spectrum alignment and quantitation based on Hierarchial Clustering Based Peak Alignment (CluPA)

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speaq-package *An R-package for NMR spectrum alignment and quantitation*

Description

Integrated NMR spectrum alignment and quantitation based on Hierarchial Clustering Based Peak Alignment (CluPA)

Details

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Author(s)

Trung Nghia VU, Kris Laukens and Dirk Valkenborg

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References

Vu TN, Valkenborg D, Smets K, Verwaest KA, Dommisse R, Lemie‘re F, Verschoren A, Goethals B, Laukens K. (2011) An integrated workflow for robust alignment and simplified quantitative analysis of NMR spectrometry data. BMC Bioinformatics. 2011 Oct 20;12:405.

BWR *BW ratio calculation*

Description

Compute the BW ratios from data groups

Usage

```
BWR(X,
    groupLabel)
```

Arguments

X	The spectral dataset in the matrix format in which each row contains a single sample
groupLabel	Group label of samples in the dataset.

Details

Compute the BW ratios from data groups

Value

Return BW ratio

Author(s)

Trung Nghia VU

See Also

createNullSampling

Examples

```
cat("\n Please see more examples in the vignettes file.")
```

---

createNullSampling *Building a null hypothesis data*

Description

Create a null sampling data (N times) and write them to a file

Usage

```
createNullSampling(X, groupLabel, N = 1000, filename = NULL, verbose=TRUE)
```

Arguments

X	The spectral dataset in the matrix format in which each row contains a single sample
groupLabel	Group label of samples in the dataset.
N	The number of iteration for creating null sample distribution
filename	The name of output file.
verbose	A boolean value to allow print out process information.

Details

Create a null sampling data (N times) and write them to a file

Author(s)

Trung Nghia VU

Examples

```
cat("\n Please see more examples in the vignettes file.")
```

`detectSpecPeaks` *Peak detection for spectra*

Description

Divide the whole spectra into smaller segments and detect peaks by using MassSpecWavelet package. Note that, the peak lists could be found by using other methods, this function is just a choice.

Usage

```
detectSpecPeaks(X, nDivRange = 128, scales = seq(1, 16, 2),
baselineThresh = 50000, SNR.Th = -1, verbose=TRUE)
```

Arguments

`X`	The spectral dataset in matrix format in which each row contains a single sample
`nDivRange`	The size of a single small segment after division of spectra
`scales`	The parameter of peakDetectionCWT function of MassSpecWavelet package, look it up in the original function.
`baselineThresh`	It will remove all peaks under an intensity set by baselineThresh.
`SNR.Th`	The parameter of peakDetectionCWT function of MassSpecWavelet package, look it up in the original function. If you set -1, the function will itseff recompute this value.
`verbose`	A boolean value to allow print out process information.

Details

Divide the whole spectra into smaller segments and detect peaks by using MassSpecWavelet package. Note that, the peak lists could be found by using other methods, this function is just a choice.

Value

The peak lists of the spectra

Author(s)

Trung Nghia VU

Examples

```
cat("\n Please see more examples in the vignettes file.")
```

dohCluster *CluPA function for multiple spectra.*

Description

Use CluPA for alignment for multiple spectra.

Usage

```
dohCluster(X,
          peakList,
          refInd = 0,
          maxShift = 100,
          acceptLostPeak = TRUE,
          verbose=TRUE)
```

Arguments

X	The spectral dataset in the matrix format in which each row contains a single sample
peakList	The peak lists of the spectra
refInd	The index of the reference spectrum.
maxShift	The maximum number of the points for a shift step.
acceptLostPeak	This is an option for users, TRUE is the default value. If the users believe that all the peaks in the peak list are true positive, change it to FALSE.
verbose	A boolean value to allow print out process information.

Details

Use CluPA for alignment for multiple spectra.

Value

The aligned spectra.

Author(s)

Trung Nghia VU

See Also

dohClusterCustommedSegments

Examples

```
cat("\n Please see more examples in the vignettes file.")
```

dohClusterCustommedSegments *Use CluPA for alignment with additional information*

Description

This function integrates some additional information from user such as references for each specific segment, segment ignorance, maximum step size.. to align spectra using CluPA.

Usage

```
dohClusterCustommedSegments(X,
                            peakList,
                            refInd,
                            maxShift,
                            acceptLostPeak = TRUE,
                            infoFilename,
                            minSegSize = 128,
                            verbose=TRUE)
```

Arguments

X	The spectral dataset in matrix format in which each row contains a single sample.
peakList	The peak lists of the spectra.
refInd	The index of the reference spectrum.
maxShift	The maximum number of points for a shift step.
acceptLostPeak	This is an option for users, TRUE is the default value. If the users believe that all the peaks in the peak list are true positive, change it to FALSE.
infoFilename	The name of the file containing the additional information from the users in the CSV format with a header.
minSegSize	The minimum size of the segments which could be considered for alignment.
verbose	A boolean value to allow print out process information.

Details

Each line of the infoFilename includes 5 numbers separated by commas, for instance:

#

begin,end,forAlign,ref,maxShift

3600,4000,0,0,0

5600,6200,1,0,50

#

- begin: the starting point of the segment.

- end: the end point of the segment.

- forAlign: the segment is aligned (1) or not (0).

- ref: the index of the reference spectrum. If 0, the algorithm will select the reference found by the reference finding step.

- maxShift: the maximum number of points of a shift to left/right.

It is worth to note that only segments with forAlign=1 will be taken into account for spectral alignment.

Value

The aligned spectral segments.

Author(s)

Trung Nghia VU

See Also

dohCluster

Examples

```
cat("\n Please see more examples in the vignettes file.")
```

---

doShift *Segment shift*

Description

Move a spectral segment of a sample shiftStep points to right or left

Usage

```
doShift(specSeg,
shiftStep)
```

Arguments

specSeg	The segment which needs to be shifted
shiftStep	The shift step for moving. If it is a negative (positive) value, the segment is moved to left (right).

Details

Move a spectral segment of a sample shiftStep points to right or left

Value

The new segment after shifting.

Author(s)

Trung Nghia VU

See Also

hClustAlign

Examples

```
cat("\n Please see more examples in the vignettes file.")
```

---

drawBW *BW and percentile ratios plot*

Description

This function is used to plot BW and percentile ratios

Usage

```
drawBW(BW,
       perc,
       X,
       startP = -1,
       endP = -1,
       groupLabel = NULL,
       highBound = -1,
       lowBound = -1,
       nAxisPos = 4,
       offside = 0)
```

Arguments

BW	An array of the BW ratios.
perc	An array of the percentile ratios.
X	The spectral dataset in matrix format in which each row contains a single sample.
startP	The starting point of the segment. If it is -1, the starting point is from begining of the spectra.
endP	The ending point of the segment. If it is -1, the ending point is the last point of the spectra.
groupLabel	The default value is NULL, it means that a single spectrum has a distinct color. Otherwise, the spectra is colored by their label.
highBound	Default value is -1, that means the plot covers also the highest intesity peaks in the figure. If the users want to limit the upper height of the figure, set this parameter by the limited value.
lowBound	Default value is -1, that means the plot covers also the lowest intesity peaks in the figure. If the users want to limit the under height of the figure, set this parameter by the limited value.
nAxisPos	The number of ticks that will be displayed in the horizontal axis.
offside	The offside of values in x-axis for display.

Details

This function is used to plot BW and percentile ratios

Author(s)

Trung Nghia VU

See Also

drawSpec

Examples

```
cat("\n Please see more examples in the vignettes file.")
```

---

drawSpec *Spectral plot*

Description

This function allows to draw a segment or the whole spectra with limited high/low bounds of intensity.

Usage

```
drawSpec(X,
         startP = -1,
        endP = -1,
        groupLabel = NULL,
        useLog = -1,
        highBound = -1,
        lowBound = -1,
        xlab = NULL,
        ylab = NULL,
        main = NULL,
        nAxisPos = 4,
        offside = 0)
```

Arguments

X	The spectral dataset in matrix format in which each row contains a single sample.
startP	The starting point of the segment. If it is -1, the starting point is from begining of the spectra.
endP	The ending point of the segment. If it is -1, the ending point is the last point of the spectra.
groupLabel	The default value is NULL, it means that a single spectrum has a distinct color. Otherwise, the spectra is colored by their label.

useLog	The default value is -1, that means do not use a logarit transformation. If users want to transform the intensities to logarit values before ploting, set it to 1.
highBound	Default value is -1, that means the plot covers also the highest intesity peaks in the figure. If the users want to limit the upper height of the figure, set this parameter by the limited value.
lowBound	Default value is -1, that means the plot covers also the lowest intesity peaks in the figure. If the users want to limit the under height of the figure, set this parameter by the limited value.
xlab	The default value is NULL, if so, "index" is displayed at the horizontal axis.
ylab	The default value is NULL, if so, "intensity" is displayed at the vertical axis.
main	The default value is NULL, if so, the title shows the values of startP and endP
nAxisPos	The number of ticks that you want to display in horizontal axis.
offside	The offside of values in x-axis for display.

Details

This function allows to draw a segment or the whole spectra with limited high/low bounds of intensity.

Author(s)

Trung Nghia VU

See Also

drawBW

Examples

```
cat("\n Please see more examples in the vignettes file.")
```

---

export2file *Export spectra to files*

Description

This function allows to export each spectrum to a single file in caMassClass format.

Usage

```
export2file(X, dirPath="./", fileList="InputFiles.csv",saveDirPath="outDir")
```

Arguments

X	The spectral dataset in matrix format in which each row contains a single sample
dirPath	The directory containing "fileList", the information files of spectra.
fileList	The name of the information file. The information file is a CSV file with header, including three columns: samplenames, label, filenames. This follows the input file format of caMassClass package.
saveDirPath	The path to the new directory containing the exported files.

Details

This function allows to export each spectrum to a single file

Author(s)

Trung Nghia VU

Examples

```
cat("\n Please see more examples in the vignettes file.")
```

`findRef` *Reference finding*

Description

This function is to heuristically detect a reference spectrum.

Usage

```
findRef(peakList)
```

Arguments

`peakList`	The peak lists of the spectra.

Details

This function is to heuristically detect a reference spectrum, see the reference for more details.

Value

`refInd`	The index of the reference spectrum found by the algorithm
`orderSpec`	A sorted array of the spectra by their goodness values

Author(s)

Trung Nghia VU

References

Vu TN, Valkenborg D, Smets K, Verwaest KA, Dommisse R, Lemie‘re F, Verschoren A, Goethals B, Laukens K. (2011) An integrated workflow for robust alignment and simplified quantitative analysis of NMR spectrometry data. BMC Bioinformatics. 2011 Oct 20;12:405.

Examples

```
cat("\n Please see more examples in the vignettes file.")
```

findSegPeakList *Selecting the peaks in a segment*

Description

This function is to find out which peaks belonging to a segment which ranges from startP to endP

Usage

```
findSegPeakList(peakList,
                startP,
                endP)
```

Arguments

peakList	The peak lists of the spectra.
startP	The starting point of the segment.
endP	The ending point of the segment.

Details

This function is to find out which peaks belonging to a segment which ranges from startP to endP

Value

The list of peaks in the segment.

Author(s)

Trung Nghia VU

See Also

dohClusterCustommedSegments

Examples

```
cat("\n Please see more examples in the vignettes file.")
```

`findShiftStepFFT` *Finding the shift-step by using Fast Fourier Transform cross-correlation*

Description

This function uses Fast Fourier Transform cross-correlation to find out the shift step between two spectra.

Usage

```
findShiftStepFFT(refSpec,
tarSpec,
maxShift = 0)
```

Arguments

`refSpec`	The reference spectrum.
`tarSpec`	The target spectrum which needs to be aligned.
`maxShift`	The maximum number of points for a shift step. If this value is zero, the algorithm will check on the whole length of the spectra.

Details

Finding the shift-step by using Fast Fourier Transform cross-correlation

Value

`corValue`	The best correlation value
`stepAdj`	The shift step found by the algorithm

Author(s)

Trung Nghia VU

See Also

`hClustAlign`

Examples

```
cat("\n Please see more examples in the vignettes file.")
```

hClustAlign *CluPA function for two spectra.*

Description

This function implements the idea of the CluPA algorithm to align the target spectrum against the reference spectrum.

Usage

```
hClustAlign(refSpec,
    tarSpec,
    peakList,
    peakLabel,
    startP,
    endP,
    distanceMethod = "average",
    maxShift = 0,
    acceptLostPeak = FALSE)
```

Arguments

refSpec	The reference spectrum.
tarSpec	The target spectrum.
peakList	List of peaks of the both reference and target spectra
peakLabel	The list of the labels of the peaks
startP	The starting point of the segment.
endP	The ending point of the segment.
distanceMethod	The distance method for the hierarchial clustering algorithm.
maxShift	The maximum number of points for a shift step.
acceptLostPeak	This is an option for users, TRUE is the default value. If the users believe that all the peaks in the peak list are true positive, change it to FALSE.

Details

This function implements the idea of the CluPA algorithm to align the target spectrum against the reference spectrum.

Value

tarSpec	The target spectrum after alignment
peakList	The peak list after alignment

Author(s)

Trung Nghia VU

References

Vu TN, Valkenborg D, Smets K, Verwaest KA, Dommisse R, Lemie‘re F, Verschoren A, Goethals B, Laukens K. (2011) An integrated workflow for robust alignment and simplified quantitative analysis of NMR spectrometry data. BMC Bioinformatics. 2011 Oct 20;12:405.

See Also

dohCluster

Examples

```
cat("\n Please see more examples in the vignettes file.")
```

---

returnLocalMaxima *Local maximum detection*

Description

Find and return local maximum of a single spectrum.

Usage

```
returnLocalMaxima(spectrum)
```

Arguments

spectrum	A spectral sample in the vector format.

Details

Find and return local maximum of a single spectrum.

Value

locMax	Locations of the found local maximum peaks
pkMax	Intensities of the found local maxumum peaks

Author(s)

Trung Nghia VU

Examples

```
cat("\n Please see more examples in the vignettes file.")
```

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