Package 'iSTATS'

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Type Package

Title A Graphical Interface to Perform STOCSY Analyses on NMR Data

Version 1.8.1

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Description Launches a 'shiny' based application for Nuclear Magnetic Resonance (NMR) data importation and Statistical TOtal Correlation SpectroscopY (STOCSY) analyses in a full interactive approach. The theoretical background and applications of the STOCSY method are described by Cloarec, O., Dumas, M. E., Craig, A., Barton, R. H., Trygg, J., Hudson, J., Blancher, C., Gauguier, D., Lindon, J. C., Holmes, E. & Nicholson, J. (2005) <doi:10.1021/ac048630x>. Spectral alignment follows the interval correlation optimized shifting method of Savorani, F., Tomasi, G. & Engelsen, S. B. (2010) <doi:10.1016/j.jmr.2009.11.012>.

Depends R(>= 3.6), shinyBS(>= 0.61), shinyWidgets(>= 0.4.3)

Imports data.table, ggplot2(>= 3.0.0), gtools(>= 3.8.1), shiny(>= 1.6.0), stats, utils

BugReports https://github.com/vitor-mendes-iq/iSTATS/issues

Encoding UTF-8

LazyData true

RoxygenNote 7.1.1

NeedsCompilation no

License GPL (>= 3)

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`CS_values_real` *Matrix of NMR chemical shifts*

Description

A matrix containing all chemical shifts of NMR data milk samples

Usage

```
CS_values_real
```

Format

A matrix with 11 rows and 32778 variables:

`file_names` *A list of sample names*

Description

A list of sample names

Usage

```
file_names
```

Format

A list of string with sample names

`icoshift` *Align Spectra with Interval Correlation Optimized Shifting*

Description

Splits spectra into intervals and rigidly shifts each interval to maximize its cross-correlation with a target. Samples must be rows and spectral points must be columns.

Usage

```
icoshift(xT, xP, inter = "whole", n = NULL, options = NULL, Scal = NULL)
```

Arguments

`xT`	A numeric target with one value per column of `xP`, or one of `"average"`, `"average2"`, `"median"`, or `"max"`. `"average2"` uses a fixed multiplier of 3.
`xP`	Numeric matrix with samples in rows and spectral points in columns.
`inter`	`"whole"`; an integer number of intervals; a character interval length or range; or a numeric vector of start/end pairs. Numeric values refer to points unless `options[5]` is 1.
`n`	Positive maximum shift, `"f"` for fast automatic search, or `"b"` for the more exhaustive search. Numeric values use points or scale units according to `options[5]`.
`options`	Numeric vector or named list with `show`, `fill`, `preCOShift`, `maxPreCOShift`, `useScal`, and `alignPreprocessed`. Defaults are `c(1, 1, 0, 0, 0, 0)`. Preprocessing values are 0 (raw), 1 (SNV), 3 (the original `msc(0, A)` behavior), -1, or -2 (derivatives).
`Scal`	Optional strictly monotonic axis with one value per column. Used for conversion when `options[5]` is 1; it is not modified.

Details

This implementation covers one-dimensional spectra, not MATLAB `icoshiftMC`. `show=2` does not create the MATLAB diagnostic plot. The `"b"` search may be slow, overlapping intervals are not reconciled, and repeated boundary filling can create edge artifacts. Character ranges use `-` as separator and cannot express negative endpoints; use numeric pairs. See `system.file("ICOSHIFT.md", package = "iSTATS")` for the app workflow.

Value

A list containing aligned matrix `xCS`, interval table `ints`, shift indices `ind` (positive is left, negative is right), and actual `target`.

References

Savorani F, Tomasi G, Engelsen SB (2010). "icoshift: A versatile tool for the rapid alignment of 1D NMR spectra." Journal of Magnetic Resonance, 202(2), 190-202. doi:10.1016/j.jmr.2009.11.012.

Examples

```
axis <- seq(1, -1, length.out = 64)
target <- dnorm(seq(-3, 3, length.out = 64))
spectra <- rbind(target, c(target[-1], 0), c(0, target[-64]))

fit <- icoshift("average", spectra, c(1, 64), n = 3,
                options = c(0, 1, 0, 0, 0, 0))
dim(fit$xCS)
fit$ind

fit_ppm <- icoshift("average", spectra, c(-0.5, 0.5), n = "f",
                    options = c(0, 1, 0, 0, 1, 1), Scal = axis)
```

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iSTATS *A Graphical Interface to Perform STOCSY analyses on NMR Data*

Description

Statistical TOtal Correlation SpectroscopY (STOCSY) is a method developed to analyze 1D Nuclear Magnetic Resonance (NMR) data, with many applications in metabolomic science, as to help the identification of molecules in complex mixture. Although STOCSY is promising method, its use requires some programming language skills. To overcome this challenge we developed the interactive STATistical Spectroscopy (iSTATS) package, based on 'shiny', in which it is possible to perform STOCSY analyses in a full interactive way, from 1D NMR matrix construction to select specifical regions to apply STOCSY methods more accurately.

Usage

```
iSTATS()
```

Value

No return value. The function is called for its side effect of launching the 'shiny' application, and returns invisibly when the application is closed.

Examples

```
if(interactive()){iSTATS::iSTATS()}
```

NMRData *Matrix of NMR intensities*

Description

A matrix containing the intensities of NMR data milk samples

Usage

```
NMRData
```

Format

A matrix with 11 rows and 32778 variables:

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