Package ‘iSTATS’

July 1, 2020

Type Package
Title A Graphical Interface to Perform STOCSY Analyses on NMR Data
Version 1.5
Date 2020-06-30
Author Luiz Henrique Keng Queiroz Junior[aut,cre], Vitor Mendes de Oliveira [aut]
Maintainer Luiz Henrique Keng Queiroz Junior <keng@ufg.br>
Description Launches a 'shiny' based application for Nuclear Magnetic Resonance (NMR) data impor-
tation and Statistical TOtal Correlation SpectroscopY (STOCSY) analyses in a full interactive
approach. The theoretical background and applica-
tions of STOCSY method could be found at Cloarec, O., Dumas, M. E., Craig, A., Bar-
ton, R. H., Trygg, J., Hudson, J., Blancher, C., Gauguier, D., Lindon, J. C., Holmes, E. & Nichol-
Depends R(>= 3.6), shinyBS(>= 0.61), shinyWidgets(>= 0.4.3)
Imports Cairo(>= 1.5), ggplot2(>= 3.0.0), gtools(>= 3.8.1), shiny(>= 1.0.2), plotly, rstudioapi, data.table
BugReports https://github.com/LaCiDIAUF/iSTATS
License GPL-3
Encoding UTF-8
LazyData true
RoxygenNote 7.1.1
NeedsCompilation no
Repository CRAN
Date/Publication 2020-07-01 12:00:11 UTC

R topics documented:

CS_values_real ................................................................. 2
file_names ................................................................. 2
iSTATS ................................................................. 2
NMRData ............................................................... 3

Index
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

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.
NMRData

Usage

iSTATS()

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:
Index

* datasets
  CS_values_real, 2
  file_names, 2
  NMRData, 3

CS_values_real, 2
file_names, 2
iSTATS, 2
NMRData, 3