Package 'mrbin'

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Title Magnetic Resonance Binning, Integration and Normalization

Version 1.4.2

Description Nuclear Magnetic Resonance is widely used in Life Science research. The package (<http://www.kleinomicslab.com/software>) converts 1D or 2D data into a matrix of values suitable for further data analysis and performs basic processing steps in a reproducible way. Negative values, a common issue in such data, are replaced by positive values. All used parameters are stored in a readable text file and can be restored from that file to enable exact reproduction of the data at a later time.

Imports grDevices, graphics, stats, utils

Depends R (>= 2.10)

License GPL-3

Encoding UTF-8

LazyData true

RoxygenNote 7.0.2.9000

Suggests

VignetteBuilder utils

NeedsCompilation no

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R topics documented:

`atnv` *A function replacing negative values.*

Description

This function replaces (column-wise) negative values by a small positive number. The number is calculated as an affine transformation to the range of the lowest positive number to 0,01*the lowest positive number (of this column). Ranks stay unchanged. Positive numbers are not altered. If sample-wise noise levels are available, the median noise level of samples with negative values is calculated and replaces the lowest positive number in case it is smaller. If no noise data is available, the 1 positive values in the data set is used as an estimate. It is recommended to us this function AFTER noise removal and other data clean-up methods, as it may alter (reduce) the noise level. If no NMR data and noise levels are provided as arguments, the function will use NMR data and noise levels from the global variables mrbin.env$bins and mrbin.env$mrbinTMP.

Usage

```
atnv(NMRdata = NULL, noiseLevels = NULL)
```

Arguments

`NMRdata`	A matrix containing NMR data. Columns=frequencies,rows=samples
`noiseLevels`	A vector

Value

NMRdata An invisible matrix containing NMR data without negative values.

Examples

```
Example<-mrbin(silent=TRUE,
                  parameters=list(verbose=TRUE,dimension="1D",PQNScaling="No",
            binwidth1D=0.005,signal_to_noise1D=1,PCA="No",binRegion=c(9.5,7.5,10,156),
                  saveFiles="No",referenceScaling="No",noiseRemoval="No",
                  fixNegatives="No",logTrafo="No",noiseThreshold=.05,
                  NMRfolders=c(system.file("extdata/2/10/pdata/10",package="mrbin"),
                             system.file("extdata/3/10/pdata/10",package="mrbin"))
                  ))
sum(Example$bins<=0)
exampleNMRpositive<-atnv(NMRdata=Example$bins, noiseLevels=Example$parameters$noise_level)
sum(exampleNMRpositive<=0)
```

`contMin` *A function for changing plotNMR plots.*

Description

This function decreases the minimum contour level of the current 2D NMR spectrum plot.

Usage

```
contMin()
```

Value

None

Examples

```
mrbin(silent=TRUE,parameters=list(dimension="2D",binwidth2D=0.5,
         binheight=3,PQNScaling="No",referenceScaling="No",binRegion=c(4,3,60,65),
         noiseRemoval="No",trimZeros="No",cropHSQC="No",
         fixNegatives="No",logTrafo="No",PCA="No",verbose=TRUE,saveFiles="No",
         NMRfolders=c(system.file("extdata/1/12/pdata/10",package="mrbin"))))
plotNMR()
contMin()
```

contPlus *A function for changing plotNMR plots.*

Description

This function increases the minimum contour level of the current 2D NMR spectrum plot.

Usage

```
contPlus()
```

Value

None

Examples

```
readBruker(folder=system.file("extdata/1/12/pdata/10",package="mrbin"),dimension="2D")
plotNMR()
contPlus()
```

cropNMR *A function for cropping HSQC spectra.*

Description

This function crops HSQC spectra to the region along the diagonal to remove uninformative signals. Will work only for 1H-13C HSQC spectra.

Usage

```
cropNMR(plot = FALSE)
```

Arguments

plot	Should a plot of the bins before and after cropping be shown? Defaults to FALSE.

Value

None

Examples

```
Example<-mrbin(silent=TRUE,
         parameters=list(dimension="2D",binwidth2D=1,binheight=4,cropHSQC="No",PCA="No",
         PQNScaling="No",noiseRemoval="No",removeSolvent="No",verbose=TRUE,
         NMRfolders=c(system.file("extdata/1/12/pdata/10",package="mrbin"))))
cropNMR()
```

down *A function for changing plotNMR plots.*

Description

This function moves down the plot region of the current NMR plot (only 2D).

Usage

```
down()
```

Value

None

Examples

```
mrbin(silent=TRUE,parameters=list(dimension="2D",binwidth2D=0.5,
         binheight=3,PQNScaling="No",referenceScaling="No",binRegion=c(4,3,60,65),
         noiseRemoval="No",trimZeros="No",cropHSQC="No",
         fixNegatives="No",logTrafo="No",PCA="No",verbose=TRUE,saveFiles="No",
         NMRfolders=c(system.file("extdata/1/12/pdata/10",package="mrbin"))))
plotNMR()
zoomIn()
down()
```

getEnv *A function for saving the package environment.*

Description

This function returns a list of all objects of the current package environment. This may be helpful for debugging or for accessing NMR spectral data and the raw bin data.

Usage

```
getEnv()
```

Value

A list containing all objects from the local package environment.

Examples

```
tempList<-getEnv()
```

intMin *A function for changing plotNMR plots.*

Description

This function decreases the intensity of the current NMR spectrum plot.

Usage

```
intMin()
```

Value

None

Examples

```
mrbin(silent=TRUE,setDefault=TRUE,parameters=list(dimension="1D",binwidth1D=.1,
         PQNScaling="No",noiseRemoval="No",trimZeros="No",
         fixNegatives="No",logTrafo="No",PCA="No",verbose=TRUE,
         NMRfolders=system.file("extdata/1/10/pdata/10",package="mrbin")))
plotNMR()
intMin()
```

intPlus *A function for changing plotNMR plots.*

Description

This function increases the intensity of the current NMR spectrum plot.

Usage

```
intPlus()
```

Value

None

Examples

```
mrbin(silent=TRUE,setDefault=TRUE,parameters=list(dimension="1D",binwidth1D=.1,
         PQNScaling="No",noiseRemoval="No",trimZeros="No",
         fixNegatives="No",logTrafo="No",PCA="No",verbose=TRUE,
         NMRfolders=system.file("extdata/1/10/pdata/10",package="mrbin")))
plotNMR()
intPlus()
```

left *A function for changing plotNMR plots.*

Description

This function moves left the plot region of the current NMR plot.

Usage

```
left()
```

Value

None

Examples

```
mrbin(silent=TRUE,parameters=list(dimension="1D",binwidth1D=.5,
         noiseRemoval="No",trimZeros="No",
         PQNScaling="No",saveFiles="No",referenceScaling="No",
         fixNegatives="No",logTrafo="No",PCA="No",verbose=TRUE,
         NMRfolders=system.file("extdata/1/10/pdata/10",package="mrbin")))
plotNMR()
zoomIn()
left()
```

logTrafo *A function for log transforming data.*

Description

This function simply log transforms. Will not work with negative data.

Usage

```
logTrafo()
```

Value

None

Examples

```
mrbinExample<-mrbin(silent=TRUE,setDefault=TRUE,parameters=list(dimension="1D", logTrafo="No",
                    binwidth1D=0.05,signal_to_noise1D=50, verbose=TRUE, PCA="No",
                    NMRfolders=c(system.file("extdata/1/10/pdata/10",package="mrbin"),
                                system.file("extdata/2/10/pdata/10",package="mrbin"))))
logTrafo()
```

mrbin *A function setting the parameters and performing binning and data processing*

Description

This function guides the user through the set-up of parameters, starts binning and performs the chosen data processing steps. If a list of parameters is provided and silent is set to TRUE, no user input is requested and binning and data processing are performed silently.

Usage

```
mrbin(silent = FALSE, setDefault = FALSE, parameters = NULL)
```

Arguments

silent	If TRUE, the user will be asked no questions and binning and data analysis will run according to the current parameters. Defaults to FALSE.
setDefault	If TRUE, all current parameters will be replaced by the default parameters (before loading any provided parameters sets). Defaults to FALSE.
parameters	Optional: A list of parameters, see examples for details. If omitted, the user will be asked through a series of question to set the parameters.

Value

An invisible list containing bins (data after processing), parameters, and factors

Examples

```
# Set parameters in command line.
mrbinExample<-mrbin(silent=TRUE,setDefault=TRUE,parameters=list(dimension="1D",
                binwidth1D=0.05,signal_to_noise1D=100,
                NMRfolders=c(system.file("extdata/1/10/pdata/10",package="mrbin"),
                             system.file("extdata/2/10/pdata/10",package="mrbin"),
                             system.file("extdata/3/10/pdata/10",package="mrbin")),
                Factors=factor(c("Group A","Group A","Group B"))))
```

plotNMR *A function for plotting NMR spectra.*

Description

This function plots the current NMR spectrum. If no parameters are provided, parameters are read from the mrbin.env environment variables, set by mrbin. To change the plot, use zoom(), zoomIn(), zoomOut(), intPlus(), intMin(), left(), right(). For 2D data use additionally: contMin(), contPlus(), up(), down()

Usage

```
plotNMR(
  region = NULL,
  rectangleRegions = NULL,
 rectangleColors = c("green", "orange", "blue", "red", "yellow", "gray", "purple"),
  rectangleFront = FALSE,
  polygonRegion = NULL,
  color = NULL,
  add = FALSE,
  showGrid = FALSE,
  manualScale = TRUE,
  plotTitle = ""
)
```

Arguments

region	A vector defining the plot region (left, right, top, bottom)
rectangleRegions	A 4-column matrix defining areas where to plot rectangles
rectangleColors	Define colors for the rectangles
rectangleFront	Plot rectangles in front of spectrum rather than in background (only 2D)
polygonRegion	Defines 4 corners of a polygon to be plotted
color	Defines the color of the spectrum plot. If NULL, a rainbow theme is used for 2D NMR
add	If TRUE, additional spectrum plots are overlaid with the current plot
showGrid	Shows a grid of data points. Defaults to FALSE
manualScale	If TRUE, scaling factor is taken from environment variables
plotTitle	Defines the main title of the plot

Value

None

Examples

```
mrbin(silent=TRUE,setDefault=TRUE,parameters=list(dimension="1D",binwidth1D=.1,
         PQNScaling="No",noiseRemoval="No",trimZeros="No",
         fixNegatives="No",logTrafo="No",PCA="No",verbose=TRUE,
         NMRfolders=system.file("extdata/1/10/pdata/10",package="mrbin")))
plotNMR()
```

plotResults *A function for plotting quality indicators, including PCA plots.*

Description

This function plots boxplots (bin-wise and sample-wise) as visual quality indicators. It also performs PCA, then plots PC1 and PC2 and loading plots.

Usage

```
plotResults()
```

Value

None

Examples

```
mrbinExample<-mrbin(silent=TRUE,setDefault=FALSE,parameters=list(dimension="2D",
                    binwidth2D=0.05,binheight=3,
                    PQNScaling="No",noiseRemoval="Yes",trimZeros="Yes",
                    fixNegatives="No",logTrafo="No",PCA="No",
                    NMRfolders=c(system.file("extdata/1/12/pdata/10",package="mrbin"),
                                 system.file("extdata/2/12/pdata/10",package="mrbin"),
                                 system.file("extdata/3/12/pdata/10",package="mrbin"))))
plotResults()
```

PQNScaling *A function for PQN scaling.*

Description

This function performs PQN scaling. To further exclude unreliable noise, only the most intense signals are used. For 1H and 1H-13C HSQC spectra, most of the sugar regions are excluded to avoid a dominating effect of the multiple sugar signals.

Usage

```
PQNScaling()
```

Value

None

Examples

```
mrbinExample<-mrbin(silent=TRUE,setDefault=TRUE,parameters=list(dimension="1D",
                    binwidth1D=0.05,PQNScaling="No",PCA="No",
                    NMRfolders=c(system.file("extdata/1/10/pdata/10",package="mrbin"),
                                 system.file("extdata/2/10/pdata/10",package="mrbin"),
                                 system.file("extdata/3/10/pdata/10",package="mrbin"))))
PQNScaling()
```

---

printParameters *A function for printing parameters to the screen.*

Description

This function reads parameters from the global variable mrbin.env$mrbinparam and prints the required R code for creating a data set to the screen.

Usage

```
printParameters()
```

Value

None

Examples

```
printParameters()
```

---

putToEnv *A function for changing and adding variables in the package environment.*

Description

This function can change variables in the current package environment. This may be helpful for debugging or for some plotting functions.

Usage

```
putToEnv(variableList)
```

Arguments

variableList	A list containing all objects to be saved in the local package environment.

Value

None

Examples

```
putToEnv(list(bins=NULL))
```

---

readBruker *A function for reading Bruker NMR spectra.*

Description

This function reads Bruker NMR data. 1D and 2D data are supported.

Usage

```
readBruker(folder = NULL, dimension = NULL, onlyTitles = FALSE)
```

Arguments

folder	Defines the exact NMR data folder. If NULL, mrbin parameter set is used
dimension	Defines the data dimension, "1D" or "2D". Only used if "folder" is not NULL
onlyTitles	Read only spectrum titles, but no data. Defaults to FALSE

Value

An (invisible) object containing spectral data

Examples

```
exampleData<-readBruker(folder=system.file("extdata/1/10/pdata/10",package="mrbin"),
                        dimension="1D")
```

---

recreatemrbin *A function recreating parameters from previous runs.*

Description

This function reads parameters from a text file that was created during a previous run or mrbin(). After reading, the data can be recreated using mrbin(). File names in mrbin$param might need to be updated. using recreatemrbin().

Usage

```
recreatemrbin(filename = NULL)
```

Arguments

filename	File path/name of the mrbin parameter file to be loaded

Value

None

Examples

```
# Insert full folder path and file name
recreatemrbin(system.file("extdata/mrbin.txt",package="mrbin"))
```

---

removeNoise *A function for removing bins below noise level.*

Description

This function checks for each bin (column) whether its level is below the individual noise level times the signal-to-noise ratio. If less than the defined threshold level are above noise*SNR, the whole bin is removed.

Usage

```
removeNoise()
```

Value

None

Examples

```
mrbin(silent=TRUE,setDefault=TRUE,parameters=list(dimension="1D",
                    binwidth1D=0.05,noiseRemoval="No",PQNScaling="No",
                    fixNegatives="No",logTrafo="No",PCA="No",verbose=TRUE,
                    NMRfolders=c(system.file("extdata/1/10/pdata/10",package="mrbin"),
                                system.file("extdata/2/10/pdata/10",package="mrbin"),
                                system.file("extdata/3/10/pdata/10",package="mrbin"))))
removeNoise()
```

resetEnv *A parameter resetting function*

Description

This function resets the parameter variables.

Usage

```
resetEnv()
```

Value

None

Examples

```
resetEnv()
```

right *A function for changing plotNMR plots.*

Description

This function moves right the plot region of the current NMR plot.

Usage

```
right()
```

Value

None

Examples

```
mrbin(silent=TRUE,parameters=list(dimension="1D",binwidth1D=.5,
         noiseRemoval="No",trimZeros="No",
         PQNScaling="No",saveFiles="No",referenceScaling="No",
         fixNegatives="No",logTrafo="No",PCA="No",verbose=TRUE,
         NMRfolders=system.file("extdata/1/10/pdata/10",package="mrbin")))
plotNMR()
zoomIn()
right()
```

setCurrentSpectrum *A function for interactively setting the current spectrum.*

Description

This function lets the user pick a spectrum from the list of spectra analysis. This function is meant only for use within the mrbin function.

Usage

```
setCurrentSpectrum(spectrumNumber = NULL)
```

Arguments

spectrumNumber	If provided, this number will be used; defaults to NULL

Value

None

Examples

```
setCurrentSpectrum(spectrumNumber=1)
```

setParam *A function setting parameters and checking for consistency.*

Description

This function set parameters and checks parameters for consistency.

Usage

```
setParam(parameters = NULL)
```

Arguments

parameters	List of parameters to be set

Value

None

Examples

```
setParam(parameters=list(dimension="1D"))
```

up *A function for changing plotNMR plots.*

Description

This function moves up the plot region of the current NMR plot (only 2D).

Usage

```
up()
```

Value

None

Examples

```
mrbin(silent=TRUE,parameters=list(dimension="2D",binwidth2D=0.5,
         binheight=3,PQNScaling="No",referenceScaling="No",binRegion=c(4,3,60,65),
         noiseRemoval="No",trimZeros="No",cropHSQC="No",
         fixNegatives="No",logTrafo="No",PCA="No",verbose=TRUE,saveFiles="No",
         NMRfolders=c(system.file("extdata/1/12/pdata/10",package="mrbin"))))
plotNMR()
zoomIn()
up()
```

zoom *A function for changing plotNMR plots.*

Description

This function changes the plot region of the current NMR plot. Can be called with no arguments: zoom(). In this case the user will be asked for manual input.

Usage

```
zoom(left = NULL, right = NULL, top = NULL, bottom = NULL)
```

Arguments

left	New left boundary
right	New right boundary
top	New top boundary
bottom	New bottom boundary

Value

None

Examples

```
mrbin(silent=TRUE,setDefault=TRUE,parameters=list(dimension="1D",binwidth1D=.1,
         PQNScaling="No",noiseRemoval="No",trimZeros="No",
         fixNegatives="No",logTrafo="No",PCA="No",verbose=TRUE,
         NMRfolders=system.file("extdata/1/10/pdata/10",package="mrbin")))
plotNMR()
zoom(left=4.6,right=2,top=10,bottom=150)
```

---

zoomIn *A function for changing plotNMR plots.*

Description

This function zooms into the plot region of the current NMR plot.

Usage

```
zoomIn()
```

Value

None

Examples

```
mrbin(silent=TRUE,setDefault=TRUE,parameters=list(dimension="1D",binwidth1D=.1,
         PQNScaling="No",noiseRemoval="No",trimZeros="No",
         fixNegatives="No",logTrafo="No",PCA="No",verbose=TRUE,
         NMRfolders=system.file("extdata/1/10/pdata/10",package="mrbin")))
plotNMR()
zoomIn()
```

---

zoomOut *A function for changing plotNMR plots.*

Description

This function zooms out from the plot region of the current NMR plot.

Usage

```
zoomOut()
```

Value

None

Examples

```
mrbin(silent=TRUE,setDefault=TRUE,parameters=list(dimension="1D",binwidth1D=.1,
         PQNScaling="No",noiseRemoval="No",trimZeros="No",
         fixNegatives="No",logTrafo="No",PCA="No",verbose=TRUE,
         NMRfolders=system.file("extdata/1/10/pdata/10",package="mrbin")))
plotNMR()
zoomIn()
zoomOut()
```

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