Package 'musicNMR'

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Title Conversion of Nuclear Magnetic Resonance spectrum in audio file

Description This package is a collection of function for converting and modifying mono dimensional nuclear magnetic resonance spectra.

Depends R (>= 2.10.0), seewave

Suggests plsgenomics

SuggestsNote No suggestions

License GPL (>= 2)

NeedsCompilation no

Repository CRAN

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R topics documented:

AU   *Collection of Free Induction Decay of Urine Spectra of the Donor AU*

Description

This dataset consists of eigth Free Induction Decay (FID) from eight urine samples. All urine were collected from the donor "AU". The urine are divided in two group; in each group urine samples were collected in a time period of a week. The collection of the two groups is separated by a time course of two years.

Usage

```
data(AU)
```

Value

A list with the following elements:

sample1A	a matrix object. FID of the sample 1 of group A.
sample2A	a matrix object. FID of the sample 2 of group A.
sample3A	a matrix object. FID of the sample 3 of group A.
sample4A	a matrix object. FID of the sample 4 of group A.
sample1B	a matrix object. FID of the sample 1 of group B.
sample2B	a matrix object. FID of the sample 2 of group B.
sample3B	a matrix object. FID of the sample 3 of group B.
sample4b	a matrix object. FID of the sample 4 of group B.

References

Assfalg M, Bertini I, Colangiuli D, *et al.*
Evidence of different metabolic phenotypes in humans.
Proc Natl Acad Sci U S A 2008;105(5):1420-4.

Examples

```
data(AU)
plotFID(AU$sample1B)
plotFID(AU$sample1A,ADD=TRUE,col=2)
```

AW	*Collection of Free Induction Decay of Urine Spectra of the Donor AU*

Description

This dataset consists of eigth Free Induction Decay (FID) from eight urine samples. All urine were collected from the donor "AW". The urine are divided in two group; in each group urine samples were collected in a time period of a week. The collection of the two groups is separated by a time course of two years.

Usage

```
data(AW)
```

Value

A list with the following elements:

sample1A   a matrix object. FID of the sample 1 of group A.

sample2A   a matrix object. FID of the sample 2 of group A.

sample3A   a matrix object. FID of the sample 3 of group A.

sample4A   a matrix object. FID of the sample 4 of group A.

sample1B   a matrix object. FID of the sample 1 of group B.

sample2B   a matrix object. FID of the sample 2 of group B.

sample3B   a matrix object. FID of the sample 3 of group B.

sample4b   a matrix object. FID of the sample 4 of group B.

References

Assfalg M, Bertini I, Colangiuli D, *et al.*
Evidence of different metabolic phenotypes in humans.
Proc Natl Acad Sci U S A 2008;105(5):1420-4.

Examples

```
data(AW)
plotFID(AW$sample1B)
plotFID(AW$sample1A,ADD=TRUE,col=2)
```

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musicMatrix   *Save an Audio File from a Matrix*

Description

This function save a matrix in audio file as *.wav

Usage

```
musicMatrix(ma,destination)
```

Arguments

ma   a matrix. The time in second unit is in the firt column. The intensity of the FID
             is in the second column.

destination Name of the .wav file

Details

This function uses - three functions from the package **tuneR**: Wave, normalize and writeWave; -
one function from the package **seewave**: savewav.

Author(s)

Stefano Cacciatore

References

Cacciatore Stefano, Edoardo Saccenti, Mario Piccioli Hypothesis: The sound of the individual
metabolic phenotype? Acoustic detection of NMR experiments OMICS: A Journal of Integrative
Biology. Submitted.

Examples

```
data(AU)
musicMatrix(AU$sample1A,"audio.wav")
```

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musicNMR	*Save an Audio File from a Bruker Nuclear Magnetic Resonance Spectrum*

Description

This function converts monodimensional Nuclear Magnetic Resonance spectrum in audio file. The spectrum is imported as Bruker format and the audio file is saved as *.wav

Usage

```
musicNMR(source,destination)
```

Arguments

source	The folder's address where the Free Induction Decay is located
destination	Name of the .wav file

Details

This function uses - three functions from the package **tuneR**: Wave, normalize and writeWave; - one function from the package **seewave**: savewav.

Author(s)

Stefano Cacciatore

References

Cacciatore Stefano, Edoardo Saccenti, Mario Piccioli Hypothesis: The sound of the individual metabolic phenotype? Acoustic detection of NMR experiments OMICS: A Journal of Integrative Biology. Submitted.

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plotFID	*Free Induction Decay Plotting*

Description

A function for ploting Free Induction Decay (FID).

Usage

```
plotFID(x,ADD=FALSE, ...)
```

Arguments

x	a matrix. The time in second unit is in the firt column. The intensity of the FID is in the second column.
ADD	For a new plot `ADD = FALSE`. To overimpose a different FID on an existing plot `ADD = TRUE`.
...	Arguments to be passed to the plot function.

Author(s)

Stefano Cacciatore

References

Cacciatore Stefano, Edoardo Saccenti, Mario Piccioli Hypothesis: The sound of the individual metabolic phenotype? Acoustic detection of NMR experiments OMICS: A Journal of Integrative Biology. Submitted.

Examples

```
data(AU)
plotFID(AU$sample1B)
plotFID(AU$sample1A,ADD=TRUE,col=2)
```

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