Package 'PepsNMRData'

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Type Package

Title Datasets for the PepsNMR package

Version 1.31.0

Suggests knitr, markdown, rmarkdown, BiocStyle

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Description This package contains all the datasets used in the PepsNMR package.

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Encoding UTF-8

LazyData true

Depends R (>= 3.5)

BugReports https://github.com/ManonMartin/PepsNMRData/issues

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Contents

`PepsNMRData-package` *Raw and (partially) pre-processed metabolomic datasets supporting the* `PepsNMR` *package*

Description

This package provides RData and Bruker files of raw and (partially) pre-processed metabolomic 1H NMR datasets from human urine and serum.

The raw Bruker files of the Human Serum are stored in the *extdata* directory of this package. They are refered as the `RawFidData_HS` dataset.

The (partially) pre-processed metabolomic 1H NMR datasets are in the form of `RData` files with the following elements:

`Data_HS_sp` 4 first FIDs and spectra of the Human Serum database after each preprocessing step.

`Data_HU_sp` 4 first FIDs and spectra of the Human Urine database after each preprocessing step.

`FidData_HS` Matrix containing the raw Free Induction Decays of the Human Serum database.

`FidData_HU` Matrix containing the raw Free Indiction Decays of the Human Urine database.

`FidInfo_HS_sp` Matrix containing acquisition parameters for the 4 first Human Serum FIDs.

`FidInfo_HS` Matrix containing acquisition parameters of the Human Serum FIDs.

`FidInfo_HU_sp` Matrix containing acquisition parameters for the 4 first Human Urine FIDs.

`FidInfo_HU` Matrix containing acquisition parameters of the Human Urine FIDs.

`FinalSpectra_HS` Matrix containing the Human Serum spectra after the full pre-treatment process.

`FinalSpectra_HU` Matrix containing the Human Urine spectra after the full pre-treatment process.

`Group_HS` Provides the group (1|2|3|4) to which belongs each signal/spectrum of the Human Serum database.

`Group_HU` Provides the group (1/2/3) to which belongs each signal/spectrum of the Human Urine database.

`RawFidData_HS` Raw Bruker files for the Human Serum datase t.

Details

Package:	PepsNMRData
Type:	Package
Version:	0.99.0
License:	GPLv2

2 different datasets are provided: Human Urine and Human Serum 1H NMR

Author(s)

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References

Rousseau, R. (2011). *Statistical contribution to the analysis of metabonomics data in 1H NMR spectroscopy* (Doctoral dissertation, PhD thesis. Institut de statistique, biostatistique et sciences actuarielles, Université catholique de Louvain, Belgium).

Martin, M., Legat, B., Leenders, J., Vanwinsberghe, J., Rousseau, R., Boulanger, B., & Govaerts, B. (2018). PepsNMR for 1H NMR metabolomic data pre-processing. *Analytica chimica acta*, 1019, 1-13.

Examples

```
# RData file
data("Data_HS_sp")

# Raw Bruker file
path <-  system.file("extdata", package = "PepsNMRData")
list.files(path)
list.dirs(path, full.names = FALSE)
```

`Data_HS_sp` *FIDs and spectra from the Human Serum database.*

Description

4 first FIDs and spectra of the Human Serum database after each preprocessing step. For more details on this database, use `help(FidData_HS)`.

Usage

```
data("Data_HS_sp")
```

Format

A list with 14 objects that are complex matrices. 4 observations/object:

`FidData_HS_0` Raw FIDs.

`FidData_HS_1` FIDs after first order phase correction.

`FidData_HS_2` FIDs after solvent residuals suppression.

`FidData_HS_3` FIDs after apodization.

`Spectrum_data_HS_4` Spectra after fourier transformation.

`Spectrum_data_HS_5` Spectra after zero order phase correction.

`Spectrum_data_HS_6` Spectra after internal calibration.

`Spectrum_data_HS_7` Spectra after baseline correction.

`Spectrum_data_HS_8` Spectra after negative values zeroing.

`Spectrum_data_HS_9` Spectra after warping.

`Spectrum_data_HS_10` Spectra after window selection.

`Spectrum_data_HS_11` Spectra after bucketing.

`Spectrum_data_HS_12` Spectra after region removal.

`Spectrum_data_HS_13` Spectra after normalization.

Source

Data provided by Dr. Pascal de Tullio and coworkers of the Pharmaceutical Chemistry Laboratory in the Pharmacy Department of the University of Liege (ULg), Belgium.

References

Rousseau, R. (2011). *Statistical contribution to the analysis of metabonomics data in 1H NMR spectroscopy* (Doctoral dissertation, PhD thesis. Institut de statistique, biostatistique et sciences actuarielles, Université catholique de Louvain, Belgium).

Examples

```
plot(Re(Data_HS_sp$FidData_HS_0[1,]), type="l")
```

Data_HU_sp *FIDs and spectra from the Human Urine database.*

Description

4 first FIDs and spectra of the Human Urine database after each preprocessing step. For more details on this database, use `help(FidData_HU)`.

Usage

```
data("Data_HU_sp")
```

Format

A list with 15 objects that are complex matrices with 4 observations/object:

`FidData_HU_0` Raw FIDs.

`FidData_HU_1` FIDs after first order phase correction.

`FidData_HU_2` FIDs after solvent residuals suppression.

`FidData_HU_3` FIDs after apodization.

`Spectrum_data_HU_4` Spectra after fourier transformation.

`Spectrum_data_HU_6` Spectra after zero order phase correction.

`Spectrum_data_HU_5` Spectra after internal calibration.

`Spectrum_data_HU_7` Spectra after baseline correction.

`Spectrum_data_HU_8` Spectra after negative values zeroing.

`Spectrum_data_HU_9` Spectra after warping.

`Spectrum_data_HU_10` Spectra after window selection.

`Spectrum_data_HU_11` Spectra after bucketing

`Spectrum_data_HU_12` Spectra after region removal.

`Spectrum_data_HU_13` Spectra after zone aggregation for the citrate peak.

`Spectrum_data_HU_14` Spectra after normalization.

Source

Data provided by Dr. Pascal de Tullio and coworkers of the Pharmaceutical Chemistry Laboratory in the Pharmacy Department of the University of Liege (ULg), Belgium.

References

Rousseau, R. (2011). *Statistical contribution to the analysis of metabonomics data in 1H NMR spectroscopy* (Doctoral dissertation, PhD thesis. Institut de statistique, biostatistique et sciences actuarielles, Université catholique de Louvain, Belgium).

Examples

```
plot(Re(Data_HU_sp$FidData_HU_0[1,]), type="l")
```

FidData_HS *Raw FIDs for the Human Serum database.*

Description

Matrix containing the raw Free Induction Decays of the Human Serum database. The experimental design is as follow: serum was collected from 4 blood donors (their class membership is available in `Group_HS`). Measurements were performed on 8 different days with replicates. The order of the measurements were permuted according to a latin hypercube sampling method.

Usage

```
data("FidData_HS")
```

Format

A complex matrix of 32 spectra with 32768 time points.

Source

Data provided by Dr. Pascal de Tullio and coworkers of the Pharmaceutical Chemistry Laboratory in the Pharmacy Department of the University of Liege (ULg), Belgium.

References

Rousseau, R. (2011). *Statistical contribution to the analysis of metabonomics data in 1H NMR spectroscopy* (Doctoral dissertation, PhD thesis. Institut de statistique, biostatistique et sciences actuarielles, Université catholique de Louvain, Belgium).

See Also

See also `FidInfo_HS` for acquisition parameters and `Group_HS` for the class of FID samples.

Examples

```
data(FidData_HS)
plot(Re(FidData_HS[1,]), type = "l")
```

FidData_HU *Raw FIDs for the Human Urine database.*

Description

Matrix containing the raw Free Indiction Decays of the Human Urine database. The experimental design is as follow: urine was collected from 3 donors (their class membership is available in `Group_HU`).

Usage

```
data("FidData_HU")
```

Format

A complex matrix of 24 spectra with 29411 time points.

Source

Data provided by Dr. Pascal de Tullio and coworkers of the Pharmaceutical Chemistry Laboratory in the Pharmacy Department of the University of Liege (ULg), Belgium.

References

Rousseau, R. (2011). *Statistical contribution to the analysis of metabonomics data in 1H NMR spectroscopy* (Doctoral dissertation, PhD thesis. Institut de statistique, biostatistique et sciences actuarielles, Université catholique de Louvain, Belgium).

See Also

See also FidInfo_HU for acquisition parameters and Group_HU for the class of FID samples.

Examples

```
data(FidData_HU)
plot(Re(FidData_HU[1,]), type = "l")
```

FidInfo_HS *Information about the FIDs for the Human Serum database.*

Description

Matrix containing acquisition parameters of the Human Serum FIDs.

Usage

```
data("FidInfo_HS")
```

Format

A matrix with 32 observations and 9 variables:

TD Time domain size

BYTORDA Determine the endiness of stored data. If 0 -> Little Endian; if 1 -> Big Endian

DIGMOD Digitization mode

DECIM Decimation rate of digital filter

DSPFVS DSP firmware version

SW_h Sweep width in Hz

SW Sweep width in ppm

O1 Spectrometer frequency offset

DT Dwell time in microseconds

Source

Data provided by Dr. Pascal de Tullio and coworkers of the Pharmaceutical Chemistry Laboratory in the Pharmacy Department of the University of Liege (ULg), Belgium.

References

Rousseau, R. (2011). *Statistical contribution to the analysis of metabonomics data in 1H NMR spectroscopy* (Doctoral dissertation, PhD thesis. Institut de statistique, biostatistique et sciences actuarielles, Université catholique de Louvain, Belgium).

See Also

See also FidData_HS for the FIDs and Group_HS for the class membership of FID samples.

Examples

```
data(FidInfo_HS)
```

FidInfo_HS_sp *Information about the 4 first Human Serum FIDs.*

Description

Matrix containing acquisition parameters for the 4 first Human Serum FIDs.

Usage

```
data("FidInfo_HS_sp")
```

Format

A matrix with 4 observations and 9 variables.

Details

Variables are:

TD Time domain size

BYTORDA The endiness of stored data. If 0 -> Little Endian; if 1 -> Big Endian

DIGMOD Digitization mode

DECIM Decimation rate of digital filter

DSPFVS DSP firmware version

SW_h Sweep width in Hz

SW Sweep width in ppm

O1 Spectrometer frequency offset

DT Dwell time in microseconds

Source

Data provided by Dr. Pascal de Tullio and coworkers of the Pharmaceutical Chemistry Laboratory in the Pharmacy Department of the University of Liege (ULg), Belgium.

References

Rousseau, R. (2011). *Statistical contribution to the analysis of metabonomics data in 1H NMR spectroscopy* (Doctoral dissertation, PhD thesis. Institut de statistique, biostatistique et sciences actuarielles, Université catholique de Louvain, Belgium).

See Also

See also Data_HS_sp for the FIDs.

Examples

```
data(FidInfo_HS)
```

`FidInfo_HU` *Information about the FIDs for the Human Urine database.*

Description

Matrix containing acquisition parameters of the Human Urine FIDs.

Usage

```
data("FidInfo_HU")
```

Format

A matrix with 24 observations and 10 variables:

TD Time domain size

BYTORDA Determine the endiness of stored data. If 0 -> Little Endian; if 1 -> Big Endian

DIGMOD Digitization mode

DECIM Decimation rate of digital filter

DSPFVS DSP firmware version

SW_h Sweep width in Hz

SW Sweep width in ppm

O1 Spectrometer frequency offset

GPRDLY Group Delay

DT Dwell time in microseconds

Source

Data provided by Dr. Pascal de Tullio and coworkers of the Pharmaceutical Chemistry Laboratory in the Pharmacy Department of the University of Liege (ULg), Belgium.

References

Rousseau, R. (2011). *Statistical contribution to the analysis of metabonomics data in 1H NMR spectroscopy* (Doctoral dissertation, PhD thesis. Institut de statistique, biostatistique et sciences actuarielles, Université catholique de Louvain, Belgium).

See Also

See also `FidData_HU` for the FIDs and `Group_HU` for the class membership of FID samples.

Examples

```
data(FidInfo_HU)
```

FidInfo_HU_sp *Information about the 4 first Human Urine FIDs.*

Description

Matrix containing acquisition parameters for the 4 first Human Urine FIDs.

Usage

```
data("FidInfo_HU_sp")
```

Format

A matrix with 4 observations and 10 variables.

Details

Variables are:

TD Time domain size

BYTORDA The endiness of stored data. If 0 -> Little Endian; if 1 -> Big Endian

DIGMOD Digitization mode

DECIM Decimation rate of digital filter

DSPFVS DSP firmware version

SW_h Sweep width in Hz

SW Sweep width in ppm

O1 Spectrometer frequency offset

GPRDLY Group Delay

DT Dwell time in microseconds

Source

Data provided by Dr. Pascal de Tullio and coworkers of the Pharmaceutical Chemistry Laboratory in the Pharmacy Department of the University of Liege (ULg), Belgium.

References

Rousseau, R. (2011). *Statistical contribution to the analysis of metabonomics data in 1H NMR spectroscopy* (Doctoral dissertation, PhD thesis. Institut de statistique, biostatistique et sciences actuarielles, Université catholique de Louvain, Belgium).

See Also

See also Data_HU_sp for the FIDs.

Examples

```
data(FidInfo_HU)
```

`FinalSpectra_HS` *Spectra for the Human Serum database after the advised preprocessing workflow.*

Description

Matrix containing the Human Serum spectra after the full pre-treatment process. At this stage the spectra are fully pre-processed. For more details on this database, see `help(FidData_HS)`.

Usage

```
data("FinalSpectra_HS")
```

Format

A complex matrix with 32 observations and 500 frequency data points in a ppm scale.

Source

Data provided by Dr. Pascal de Tullio and coworkers of the Pharmaceutical Chemistry Laboratory in the Pharmacy Department of the University of Liege (ULg), Belgium.

References

Rousseau, R. (2011). *Statistical contribution to the analysis of metabonomics data in 1H NMR spectroscopy* (Doctoral dissertation, PhD thesis. Institut de statistique, biostatistique et sciences actuarielles, Université catholique de Louvain, Belgium).

See Also

See also `FidData_HS` for the raw FIDs and `Group_HS` for the samples class.

Examples

```
data(FinalSpectra_HS)
plot(Re(FinalSpectra_HS[1,]), type="l")
```

`FinalSpectra_HU` *Spectra for the Human Urine database after the advised preprocessing workflow.*

Description

Matrix containing the Human Urine spectra after the full pre-treatment process. At this stage the spectra are fully pre-processed.

Usage

```
data("FinalSpectra_HU")
```

Format

A complex matrix with 24 observations and 500 frequency data points in a ppm scale.

Source

Data provided by Dr. Pascal de Tullio and coworkers of the Pharmaceutical Chemistry Laboratory in the Pharmacy Department of the University of Liege (ULg), Belgium.

References

Rousseau, R. (2011). *Statistical contribution to the analysis of metabonomics data in 1H NMR spectroscopy* (Doctoral dissertation, PhD thesis. Institut de statistique, biostatistique et sciences actuarielles, Université catholique de Louvain, Belgium).

See Also

See also `FidData_HU` for the raw FIDs and `Group_HU` for the samples class.

Examples

```
data(FinalSpectra_HU)
plot(Re(FinalSpectra_HU[1,]), type="l")
```

Group_HS *Class of Human Serum spectra.*

Description

Provides the group (1|2|3|4) to which belongs each signal/spectrum of the Human Serum database. For more details on this database, see `help(FidData_HS)`.

Usage

```
data("Group_HS")
```

Format

A vector of length 32.

Source

Data provided by Dr. Pascal de Tullio and coworkers of the Pharmaceutical Chemistry Laboratory in the Pharmacy Department of the University of Liege (ULg), Belgium.

References

Rousseau, R. (2011). *Statistical contribution to the analysis of metabonomics data in 1H NMR spectroscopy* (Doctoral dissertation, PhD thesis. Institut de statistique, biostatistique et sciences actuarielles, Université catholique de Louvain, Belgium).

See Also

See also `FidInfo_HS` for acquisition parameters and `FidData_HS` for the FIDs.

Examples

```
data(Group_HS)
```

Group_HU *Class of Human Urine spectra.*

Description

Provides the group (1/2/3) to which belongs each signal/spectrum of the Human Urine database.

Usage

```
data("Group_HU")
```

Format

A vector of length 24.

Source

Data provided by Dr. Pascal de Tullio and coworkers of the Pharmaceutical Chemistry Laboratory in the Pharmacy Department of the University of Liege (ULg), Belgium.

References

Rousseau, R. (2011). *Statistical contribution to the analysis of metabonomics data in 1H NMR spectroscopy* (Doctoral dissertation, PhD thesis. Institut de statistique, biostatistique et sciences actuarielles, Université catholique de Louvain, Belgium).

See Also

See also FidInfo_HU for acquisition parameters and FidData_HU for the FIDs.

Examples

```
data(Group_HU)
```

RawFidData_HS *Raw Bruker files for the Human Serum dataset.*

Description

Contains the Bruker files for the 32 spectra of the Human Serum dataset.

Usage

```
data("RawFidData_HS")
```

Format

The *inst/extdata* directory contains a series of sub-directories, one by FID.

Source

Data provided by Dr. Pascal de Tullio and coworkers of the Pharmaceutical Chemistry Laboratory in the Pharmacy Department of the University of Liege (ULg), Belgium.

References

Martin, M., Legat, B., Leenders, J., Vanwinsberghe, J., Rousseau, R., Boulanger, B., & Govaerts, B. (2018). PepsNMR for 1H NMR metabolomic data pre-processing. *Analytica chimica acta*, 1019, 1-13.

Examples

```
# Raw Bruker file
path <-  system.file("extdata", package = "PepsNMRData")
list.files(path)
list.dirs(path, full.names = FALSE)
```

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