# Package 'PepsNMRData'

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**Type** Package

**Title** Datasets for the PepsNMR package

**Version** 1.26.0

**Suggests** knitr, markdown, rmarkdown, BiocStyle

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

**License** GPL-2 | file LICENSE

**Encoding** UTF-8

**LazyData** true

**Depends** R (>= 3.5)

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

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

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## 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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Maintainer: Manon Martin <manon.martin@uclouvain.be>

## 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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