

# Package ‘PepsNMRData’

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**Title** Datasets for the PepsNMR package

**Version** 1.21.0

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

**Contact** Manon Martin <manon.martin@uclouvain.be>, Bernadette Govaerts  
<bernadette.govaerts@uclouvain.be> or Benoît Legat  
<benoit.legat@gmail.com>

**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>

**biocViews** ExperimentData, OrganismData, Homo\_sapiens\_Data

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**Author** Manon Martin [aut, cre],  
Bernadette Govaerts [aut, ths],  
Pascal de Tullio [dct]

**Maintainer** Manon Martin <manon.martin@uclouvain.be>

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PepsNMRData-package	<i>Raw and (partially) pre-processed metabolomic datasets supporting the PepsNMR package</i>
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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 referred 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 Induction 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 dataset.

## 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)

Benoît Legat, Bernadette Govaerts & Manon Martin

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 Induction 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 endianness 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 endianness 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)
```

**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 endianness 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 endianness 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	<i>Spectra for the Human Serum database after the advised preprocessing workflow.</i>
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---

### 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	<i>Spectra for the Human Urine database after the advised preprocessing workflow.</i>
-----------------	---------------------------------------------------------------------------------------

---

### 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	<i>Class of Human Serum spectra.</i>
----------	--------------------------------------

---

**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	<i>Class of Human Urine spectra.</i>
----------	--------------------------------------

---

**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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