

# Package ‘nmrdata’

May 5, 2026

**Type** Package

**Title** Example 1d NMR Data for Metabolic Profiling

**Version** 1.3.0

**Description** Provides example one-dimensional proton NMR spectra of murine urine samples collected before and after bariatric or sham surgery (Roux-en-Y gastric bypass). The data are adapted from Jia V Li et al. (2011), “Metabolic surgery profoundly influences gut microbial-host metabolic cross-talk”, *Gut*, 60(9), 1214–1223. <[doi:10.1136/gut.2010.234708](https://doi.org/10.1136/gut.2010.234708)>. This package serves as example data for metabolomics analysis and teaching purposes.

**License** MIT + file LICENSE

**Encoding** UTF-8

**LazyData** false

**Roxygen** list(markdown = TRUE)

**RoxygenNote** 7.3.3

**Imports** ExperimentHub,

**Suggests** BiocStyle, knitr, rmarkdown

**VignetteBuilder** knitr

**biocViews** ExperimentHub, ExperimentData

**BugReports** <https://github.com/tkimhofer/nmrdata/issues>

**URL** <https://github.com/tkimhofer/nmrdata>

**git\_url** <https://git.bioconductor.org/packages/nmrdata>

**git\_branch** devel

**git\_last\_commit** 204a85d

**git\_last\_commit\_date** 2026-04-28

**Repository** Bioconductor 3.24

**Date/Publication** 2026-05-05

**Author** Torben Kimhofer [aut, cre] (ORCID:  
<<https://orcid.org/0000-0001-7158-9930>>)

**Maintainer** Torben Kimhofer <[tkimhofer@gmail.com](mailto:tkimhofer@gmail.com)>

## Contents

getRawExpDir . . . . .	2
nmrdata . . . . .	3
<b>Index</b>	<b>4</b>

---

getRawExpDir	<i>Unpack and return path to raw NMR experiment directory</i>
--------------	---

---

### Description

Retrieves the raw NMR experiment archive (tar.gz) from ExperimentHub and ensures it is unpacked once into a cache directory. If the unpacked directory already exists and contains files, it is reused; otherwise the tarball is extracted. Optionally, an existing unpack can be forced to be replaced.

### Usage

```
getRawExpDir(quiet = FALSE, reuntar = FALSE, tar_override = NULL)
```

### Arguments

quiet	Logical; suppress progress messages (default FALSE).
reuntar	Logical; force re-extraction even if the directory already exists and is populated (default FALSE).
tar_override	Character path to a local .tar.gz file to use instead of ExperimentHub (for examples/tests; default NULL).

### Details

This helper is idempotent: repeated calls return the same normalized path without re-downloading or re-unpacking, unless explicitly instructed.

- The function always uses the same internal ExperimentHub ID (EH9906 by default in this package).
- The tarball is retrieved via `ExperimentHub::ExperimentHub()`.
- The directory is created next to the cached tarball inside the EH cache.
- If the archive contains exactly one top-level folder, that name is reused. Otherwise a default folder name ("nmrdata") is created.

### Value

A character scalar: normalized absolute path to the unpacked dataset directory inside the local ExperimentHub cache.

### See Also

`ExperimentHub::ExperimentHub()`, `utils::untar()`

## Examples

```
td <- tempfile(); dir.create(td)
dir.create(file.path(td, "tinydata"))
cat("ex data\n", file = file.path(td, "tinydata", "a.txt"))
tarfile <- file.path(td, "tinydata.tar.gz")
utils::tar(tarfile, files = "tinydata", compression = "gzip", tar = "internal")

p <- getRawExpDir(tar_override = tarfile, quiet = TRUE)
basename(p)           # "tinydata"
list.files(p)         # "a.txt"

## Not run:
exp_dir <- getRawExpDir()
list.files(exp_dir, recursive = TRUE)[1:5]

# Force re-unpack if you think the folder is corrupted
exp_dir <- getRawExpDir(reuntar = TRUE)

## End(Not run)
```

---

nmrdata

*nmrdata: Example 1D NMR Data for Metabolic Profiling*

---

## Description

The **nmrdata** package provides example one-dimensional proton NMR spectra intended for code development and teaching in a metabolomics framework.

## Details

Two resources are available:

- a **pre-processed dataset** for prototyping spectral and statistical analyses,
- **raw Bruker experiment folders** for I/O and processing demonstrations.

For further details, see the [nmrdata vignette](#).

## Author(s)

**Maintainer:** Torben Kimhofer <[tkimhofer@gmail.com](mailto:tkimhofer@gmail.com)> ([ORCID](#))

## See Also

Useful links:

- <https://github.com/tkimhofer/nmrdata>
- Report bugs at <https://github.com/tkimhofer/nmrdata/issues>

# Index

\* **internal**

nmrdata, 3

ExperimentHub::ExperimentHub(), 2

getRawExpDir, 2

nmrdata, 3

nmrdata-package (nmrdata), 3

utils::untar(), 2