# Package 'nmrdata'

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**Type** Package

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

**Version** 1.2.0

**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>. This package serves as example data for metabolomics analysis and teaching purposes.

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**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

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# Contents



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`getRawExpDir` *Unpack and return path to raw NMR experiment directory*

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## 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)
```

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

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## 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> (ORCID)

## See Also

Useful links:

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

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