Package 'nmrdata'

October 27, 2026

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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Imports ExperimentHub,

Suggests BiocStyle, knitr, rmarkdown

VignetteBuilder knitr

biocViews ExperimentHub, ExperimentData

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

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)

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See Also

Useful links:

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

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