Package 'ptairData'

November 10, 2026

Title PTR-TOF-MS volatolomics raw datasets from exhaled air and cell culture headspace

Version 1.20.0

Description The package ptairData contains two raw datasets from Proton-Transfer-Reaction Time-of-Flight mass spectrometer acquisitions (PTR-TOF-MS), in the HDF5 format. One from the exhaled air of two volunteer healthy individuals with three replicates, and one from the cell culture headspace from two mycobacteria species and one control (culture medium only) with two replicates. Those datasets are used in the examples and in the vignette of the ptairMS package (PTR-TOF-MS data pre-processing). There are also used to gererate the ptrSet in the ptairMS data : exhaledPtrset and mycobacteriaSet

License GPL-3

Encoding UTF-8

RoxygenNote 7.1.1

BugReports https://github.com/camilleroquencourt/ptairData/issues

biocViews ExperimentData, MassSpectrometryData, CellCulture

Suggests knitr, rmarkdown, testthat, BiocStyle

VignetteBuilder knitr

Imports rhdf5, signal, stats, graphics

git_url https://git.bioconductor.org/packages/ptairData

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Contents

ptairData-package 2

Index **3**

`ptairData-package` *ptairData: PTR-TOF-MS volatolomics raw datasets from exhaled air and cell culture headspace*

Description

The package ptairData contains two raw datasets from Proton-Transfer-Reaction Time-of-Flight mass spectrometer acquisitions (PTR-TOF-MS), in the HDF5 format: one from the exhaled air of two volunteer healthy individuals, and one from the cell culture headspace from two mycobacteria species and one control (culture medium only). Those datasets are used in the examples and in the vignette from the ptairMS package (PTR-TOF-MS data pre-processing).

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Index

∗ **internal**
ptairData-package, 2

ptairData *(*ptairData-package*)*, 2
ptairData-package, 2