## Package 'ptairData'

November 21, 2024

Proton-Transfer-Reaction Time-of-Flight mass spectrometer acquisitions (PTR-TOF-MS),

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

in the HDF5 format. One from the exhaled air of two volunteer healthy

Description The package ptairData contains two raw datasets from

culture headspace

**Version** 1.14.0

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	
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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).

## Author(s)

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