Package 'ptairData'

November 12, 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 | |
| git_url https://git.bioconductor.org/packages/ptairData | |
| git_branch RELEASE_3_20 | |
| git_last_commit aedc601 | |
| git_last_commit_date 2024-10-29 | |
| Repository Bioconductor 3.20 | |
| Date/Publication 2024-11-12 | |
| Author camille Roquencourt [aut, cre] | |
| Maintainer camille Roquencourt < camille.roquencourt@hotmail.fr> | |
| Contents | |
| ptairData-package | - |
| Index | • |

2 ptairData-package

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)

Maintainer: camille Roquencourt < camille.roquencourt@hotmail.fr>

Index

```
* internal
    ptairData-package, 2

ptairData (ptairData-package), 2
ptairData-package, 2
```