Package 'RMassBankData'

March 11, 2025

Type Package

Title Test dataset for RMassBank

Version 1.44.0

Author Michael Stravs, Emma Schymanski, Steffen Neumann

Maintainer Michael Stravs, Emma Schymanski <massbank@eawag.ch>

Description Example spectra, example compound list(s) and an example annotation list for a narcotics dataset; required to test RMassBank. The package is described in the man page for RMassBankData. Includes new XCMS test data.

biocViews ExperimentData, MassSpectrometryData

License Artistic-2.0

Suggests RMassBank

Collate 'RMassBankData.R'

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

git_branch RELEASE_3_20

git_last_commit f0dab4e

git_last_commit_date 2024-10-29

Repository Bioconductor 3.20

Date/Publication 2025-03-11

Contents

RMassBankData	*RMassBank test dataset*

Description

This contains data suitable to test the RMassBank functionalities.

Details

The package contains the folders:

- spectra LC-MS runs of 15 narcotics standards, in mzML format and deprofiled.
- listA CSV list with compound informations for the 15 narcotics, as needed by RMassBank.
- infolistsA complete CSV list with annotations for the 15 standards.
- infolists_incompleteA partial list of `infolists`, to demonstrate the download of missing entries.
- infolists_editedThe downloaded missing entries, subsequently checked and completed by hand.
- resultsThe intermediate and final results of the `msms_workflow` runs. This serves to build the vignette, since it would take too long to run the whole workflow during the vignette build.

Author(s)

Michael Stravs, Eawag <michael.stravs@eawag.ch

Index