

Package ‘RMassBankData’

December 19, 2024

Type Package

Title Test dataset for RMassBank

Version 1.45.0

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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 devel

git_last_commit 98941db

git_last_commit_date 2024-10-29

Repository Bioconductor 3.21

Date/Publication 2024-12-19

Contents

RMassBankData	2
Index	3

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.

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Index

- * **datasets**

- RMassBankData, [2](#)

- * **data**

- RMassBankData, [2](#)

- RMassBankData, [2](#)