

Package ‘RMassBankData’

April 13, 2017

Type Package

Title Test dataset for RMassBank

Version 1.12.0

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'

NeedsCompilation no

R topics documented:

RMassBankData 1

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_edited` The downloaded missing entries, subsequently checked and completed by hand.
- `results` The 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

*Topic **datasets**

RMassBankData, [1](#)

*Topic **data**

RMassBankData, [1](#)

RMassBankData, [1](#)