

Package ‘RMassBankData’

April 8, 2015

Type Package

Title Test dataset for RMassBank

Version 1.3.1

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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'

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RMassBankData	<i>RMassBank test dataset</i>
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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.

- `infolists`A complete CSV list with annotations for the 15 standards.
- `infolists_incomplete`A 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.

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