Package 'RMassBankData'

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Type Package

Title Test dataset for RMassBank

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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 *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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