Package 'RMassBankData'

October 16, 2018

Title Test dataset for RMassBank Version 1.18.0 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_7 git_last_commit_date 2018-04-30 Date/Publication 2018-10-16 R topics documented: RMassBankData RMassBankData RMassBankData RMassBankData RMassBankData</massbank@eawag.ch>	Type Package	
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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.
- 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)

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