

# Package ‘RMassBankData’

April 14, 2020

**Type** Package

**Title** Test dataset for RMassBank

**Version** 1.24.0

**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\_10

**git\_last\_commit** b9bd233

**git\_last\_commit\_date** 2019-10-29

**Date/Publication** 2020-04-14

## R topics documented:

RMassBankData	1
<b>Index</b>	<b>3</b>

---

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

---

## 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)**

Michael Stravs, Eawag <michael.stravs@eawag.ch

# Index

\*Topic **datasets**

RMassBankData, [1](#)

\*Topic **data**

RMassBankData, [1](#)

RMassBankData, [1](#)