

# Package ‘RMassBankData’

October 17, 2024

**Type** Package

**Title** Test dataset for RMassBank

**Version** 1.42.0

**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\_19

**git\_last\_commit** 5a660a0

**git\_last\_commit\_date** 2024-04-30

**Repository** Bioconductor 3.19

**Date/Publication** 2024-10-17

## Contents

RMassBankData . . . . .	2
<b>Index</b>	<b>3</b>

---

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.

### **Author(s)**

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

# Index

- \* **datasets**

- RMassBankData, [2](#)

- \* **data**

- RMassBankData, [2](#)

- RMassBankData, [2](#)