

# Package ‘RMassBankData’

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**Type** Package

**Title** Test dataset for RMassBank

**Version** 1.39.0

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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'

**git\_url** <https://git.bioconductor.org/packages/RMassBankData>

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RMassBankData

*RMassBank test dataset*

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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.

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