

# Package ‘msPurityData’

October 12, 2020

**Type** Package

**Title** Fragmentation spectral libraries and data to test the msPurity package

**Version** 1.16.0

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**Description** Fragmentation spectral libraries and data to test the msPurity package

**License** GPL (>= 2)

**LazyData** TRUE

**VignetteBuilder** knitr

**RoxygenNote** 5.0.1

**Suggests** knitr

**biocViews** ExperimentData, MassSpectrometryData

**NeedsCompilation** no

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

**git\_branch** RELEASE\_3\_11

**git\_last\_commit** 62a9546

**git\_last\_commit\_date** 2020-04-27

**Date/Publication** 2020-10-12

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msPurityData-package    *Test data for the msPurity package*

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### **Description**

This data package contains test data to be used with package msPurity, see folders lcms and dims. This contains LC-MS, LC-MS/MS and DI-MS datasets in mzML format. There are also various .csv files and .rds files representing model outputs from the msPurity package. The LC-MS, LC-MS/MS and DI-MS datasets have been reduced in size by reducing the number of scans and m/z range.

The data package also contains a fragmentation spectral library created by msp2db (<https://msp2db.readthedocs.io/en/latest/>) with data from MassBank, GNPS, LipidBlast and HMDB. This is the default spectral library that is used with the spectral\_matching with msPurity. The library data is from MoNA (<http://mona.fiehnlab.ucdavis.edu/download/>) downloaded on 5th November 2018.

The dataset also contains data relating to the msPurity publication.

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