

# Package ‘msPurityData’

May 15, 2025

**Type** Package

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

**Version** 1.37.0

**Date** 12-12-2018

**Author** Thomas N. Lawson

**Maintainer** Thomas N. Lawson <thomas.nigel.lawson@gmail.com>

**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** devel

**git\_last\_commit** 2392aad

**git\_last\_commit\_date** 2025-04-15

**Repository** Bioconductor 3.22

**Date/Publication** 2025-05-15

## Contents

msPurityData-package . . . . .	2
<b>Index</b>	<b>3</b>

---

msPurityData-package    *Test data for the msPurity package*

---

### **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.

# Index

`msPurityData` (`msPurityData-package`), [2](#)  
`msPurityData-package`, [2](#)