

Package ‘msPurityData’

October 12, 2023

Type Package

Title Fragmentation spectral libraries and data to test the msPurity package

Version 1.28.0

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 RELEASE_3_17

git_last_commit f45a1dd

git_last_commit_date 2023-04-25

Date/Publication 2023-10-12

R topics documented:

msPurityData-package 2

Index 3

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/downloads/>) downloaded on 5th November 2018.

The dataset also contains data relating to the msPurity publication.

Index

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