Package ‘msPurityData’

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Type Package

Title Fragmentation spectral libraries and data to test the msPurity package

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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

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Contents

`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/late 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/downlo downloaded on 5th November 2018.

The dataset also contains data relating to the msPurity publication.

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