Package 'msdata'

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Title Various Mass Spectrometry raw data example files

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Suggests xcms

ZipData no

Description Ion Trap positive ionization mode data in mzData file format.
Subset from 500-850 m/z and 1190-1310 seconds, incl. MS2 and MS3,intensity threshold 100.000. Extracts from FTICR Apex III, m/z 400-450.
Subset of UPLC - Bruker micrOTOFq data, both mzData and mzML.

biocViews ExperimentData, MassSpectrometryData

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R topics documented:

| msdata | *Sample FTICR, LC/MS and MS^n data* |

Description

x object containing a subset of LC/MS raw data from a Thermo Finnigan LCQ Deca XP The data is a subset from 500-850 m/z and 1190-1310 seconds, incl. MS2 and MS3, intensity threshhold 100.000. It was collected in positive ionization mode.

xs object containing a subset of FTICR data from a Bruker APex III FTICR. The data is a subset from 400-450 m/z, collected in positive ionization mode.

Usage

    data(xs)

Format

The format is:

    xs

Details

The corresponding raw mzdata files are located in the fticr and iontrap subdirectory of this package.

See Also

xcmsSet, xcmsRaw

Examples

```
## The directory with the mzData LC/MS files
data(xs)
mzdatapath <- file.path(.find.package("msdata"), "iontrap")
mzdatapath
files <- list.files(mzdatapath, recursive = TRUE, full.names = TRUE)
files

if (require(xcms)) {

## xcmsSet Summary
show(xs)

## Access raw data file
x <- xcmsRaw(files[1])
x

}
```

Index