Package 'msdata'

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Title Various Mass Spectrometry raw data example files

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Suggests xcms, mzR

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, mzML and mz5. LC-MSMS and MRM files from proteomics experiments. PSI mzIdentML example files for various search engines.

biocViews ExperimentData, MassSpectrometryData

License GPL (>= 2)

NeedsCompilation no

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

}
```

`proteomics` *Proteomics data in* `msdata`

Description

This function returns proteomics mass spectrometry files. These files are all stored in the `proteomics` directory in the `msdata` package. Each file/data is described in more details below.

Usage

```
proteomics(...)
```

Arguments

`...`	Additional arguments passed to `list.files`.

Details

- `TMT_Erwinia_1uLSike_Top10HCD_isol2_45stepped_60min_01.mzML.gz`: A LC-MSMS data file containing iTRAQ 4-plex data. The data is described in more details in Gatto L. and Christoforou A. *Using R and Bioconductor for proteomics data analysis* (PMID 23692960). This file only contains a subset of the fill data (spectra 1002 to 1510) and was generated from the full data using `msconvert` (ProteoWizard release: 3.0.9283 (2016-1-11)) using following command

  ```
  msconvert TMT_Erwinia_1uLSike_Top10HCD_isol2_45stepped_60min_01-20141210.mzML
  --filter "index [1002,1510]" -o subset
  ```

  The original file is available in the ProteomeXchange `PXD000001` project.

  An MS2 identification file, `ident/TMT_Erwinia_1uLSike_Top10HCD_isol2_45stepped_60min_01-20141210.m` generated searching the raw data against the *Erwinia carotovora* database (see reference above) is also available through the `ident` function.

- `MS3TMT10_01022016_32917-33481.mzML.gz`:A subset of 565 spectra from a currenly unpublished TMT 10-plex experiment run on an Thermo Orbitrap Lumos with synchronous precursor selection (SPS) MS3. Only the MS2 spectra were centroided during convertion using `msconvert` (ProteoWizard release: 3.0.9283 (2016-1-11)) using vendor libraries.
- MRM-standmix-5.mzML.gz:Sample from mouse brain acquired by HILIC ESI-QqQ/MS in Dynamic multiple reaction monitoring mode (MRM). HPLC system was a 1290 Infinity (Agilent Technologies) coupled to ion-Funnel Triple quadrupole 6490 mass spectrometer (Agilent Technologies). This file was contributed by Xavi Domingo-Almenara from theThe Scripps Research Institute, San Diego, CA.

Value

A `character` with file names.

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See Also

For more access to mass spectrometry-based proteomics data, see the `rpx` and `ProteomicsAnnotationHubData` packages.

Examples

```
(f <- proteomics(full.names = TRUE))

library(mzR)
openMSfile(f[2])
```

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