Package 'msdata'

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Title Various Mass Spectrometry raw data example files

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Depends R (>= 2.10)

Suggests xcms, mzR, MSnbase

ZipData no

Description Ion Trap positive ionization mode data in mzML 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 mzML and mz5. LC-MSMS and MRM files from proteomics experiments. PSI mzIdentML example files for various search engines.

biocViews ExperimentData, MassSpectrometryData

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Contents

CE-MS *CE-MS test data*

Description

The CE-MS test files consist of two files, i.e. `"CEMS_10ppm.mzML"` and `"CEMS_25ppm.mzML"`. The data contains CE-MS runs of a standard mixture that contains e.g. Lysine (at 10 ppm and 25 ppm, respectively) and the neutral EOF marker Paracetamol (50 ppm). The data was acquired on a 7100 capillary electrophoresis system from Agilent Technologies, coupled to an Agilent 6560 IM-QToF-MS. CE Separation was performed using a 80 cm fused silica capillary with an internal diameter of 50 µm and external diameter of 365 µm. The Background Electrolyte was 10 % acetic acid and separation was performed at +30 kV and a constant pressure of 50 mbar. MS detection was performed in positive ionization mode.

The raw data were then converted to an open-source ".mzML" format (Proteowizzard) and load into R via the `MSnBase::readMSData()` function. In order to reduce data size, the test data was subsequently cutted in migration time and mz range using `filterRt(rt = c(400, 900))` and `filterMz(mz = c(147.1, 152.0))` from `MSnBase`

Author(s)

Liesa Salzer

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 mzML files are located in the `fticr-mzML` and `iontrap` subdirectory of this package.

See Also

xcmsSet, xcmsRaw

Examples

```
## The directory with the mzML LC/MS files
data(xs)
mzMLpath <- file.path(find.package("msdata"), "iontrap")
mzMLpath
files <- list.files(mzMLpath, 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 TMT6 6-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 complete file is `TMT_Erwinia_1uLSike_Top10HCD_isol2_45stepped_60min_01-20141210.mzML.gz`, also available here, and can also be downloaded from the ProteomeXchange `PXD000001` project (see the `rpx` package).

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.
- MS3TMT11.mzML:A subset of 994 spectra from a currenly unpublished MS3 SPS TMT 11-plex experiment converted to mzML using msconvert. The file contains 30, 482 and 482 MS1, MS2 and MS3 spectra, respectively. The MS1 spectra are in profile mode; other MS levels are centroided. See *Sensitive and Accurate Quantitation of Phosphopeptides Using TMT Isobaric Labeling Technique* for details about the acquisition method.

  An feature data containing identification data is available with data(fdms3tmt11), which can be used to directly update the feature data, as shown in the example below.
- 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.

Author(s)

Laurent Gatto <laurent.gatto@uclouvain.be>

See Also

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

Examples

```
## raw data files
(f <- proteomics(full.names = TRUE))

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

library("MSnbase")
## The MS3 TMT11 raw data
(fms3 <- proteomics(full.names = TRUE, pattern = "MS3TMT11.mzML"))
ms3 <- readMSData(fms3, mode = "onDisk")
ms3

## Additional feature metadata
data(fdms3tmt11)
names(fdms3tmt11)

fData(ms3) <- fdms3tmt11
validObject(ms3)
```

```
## identification data file
ident(full.names = TRUE)

## quantiative data files
quant(full.names = TRUE)
```

`sciexdata` *AB Sciex LC-MS data files*

Description

The mzML files in the `sciex` directory in the `msdata` package represent profile-mode LC-MS data of pooled human serum samples (the same pool being measured). The samples were analyzed by ultra high-performance liquid chromatography (UHPLC; Agilent 1290) coupled to a Q-TOF mass spectrometer (TripleTOF 5600+ AB Sciex). The chromatographic separation was based in hydrophilic interaction liquid chromatography (HILIC) and performed using an Waters Acquity BEH Amide, 100 x 2.1 mm column.

The mass specctrometer was operated in full scan mode in the mass range from 50 to 1000 m/z and with an accumulation time of 250 ms. The files represent a subset of spectra/scans from m/z 105 to 134 and from retention time 0 to 260 seconds. The files were generated in the same LC-MS run, but from different injections. Details on the individual files are provided below.

Details

- 20171016_POOL_POS_1_105-134.mzML profile-mode LC-MS data of pooled human serum samples. Injection index: 1.
- 20171016_POOL_POS_3_105-134.mzML profile-mode LC-MS data of pooled human serum samples. Injection index: 19.

Author(s)

Sigurdur Smarason, Giuseppe Paglia and Johannes Rainer

Examples

```
## List the files in the sciex folder
dir(system.file("sciex", package = "msdata"))
```

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