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.

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License GPL (>= 2)

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`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`.

Value

A `character` with file names.

Author(s)

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See Also

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

`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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