

msdata

March 23, 2012

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Sample FTICR, LC/MS and MSⁿ 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 threshold 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

*Topic **datasets**

[msdata](#), [1](#)

[msdata](#), [1](#)

[x \(msdata\)](#), [1](#)

[xcmsRaw](#), [1](#)

[xcmsSet](#), [1](#)

[xs \(msdata\)](#), [1](#)