msdata

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Sample FTICR, LC/MS and MS\$^n\$ data

Description

 \times 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
mzdatapath <- file.path(.find.package("msdata"), "iontrap")
mzdatapath
files <- list.files(mzdatapath, recursive = TRUE, full.names = TRUE)
if (require(xcms)) {</pre>
```

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```
## xcmsSet Summary
show(xs)

## Access raw data file
x <- xcmsRaw(files[1])
x
}</pre>
```

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