

# Package ‘msdata’

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**Version** 0.10.0

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**Title** Various Mass Spectrometry raw data example files

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**Suggests** xcms

**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. PSI mzIdentML example files for various search engines.

**biocViews** ExperimentData, MassSpectrometryData

**License** GPL (>= 2)

**NeedsCompilation** no

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

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## 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

}
```

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