

# Package ‘msdata’

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**Version** 0.14.0

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

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**Suggests** xcms, mzR

**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. LC-MSMS files from proteomics experiments. PSI mzIdentML example files for various search engines.

**biocViews** ExperimentData, MassSpectrometryData

**License** GPL (>= 2)

**NeedsCompilation** no

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msdata	<i>Sample FTICR, LC/MS and MS<sup>n</sup> data</i>
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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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proteomics

*Proteomics data in msdata*

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## 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 iTRAQ 4-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 full 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 original file is available in the ProteomeXchange PXD000001 project.

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 currently unpublished TMT 10-plex experiment run on an Thermo Orbitrap Lumos with synchronous precursor selection (SPS) MS3. Only the MS2 spectra were centroided during conversion using msconvert (ProteoWizard release: 3.0.9283 (2016-1-11)) using vendor libraries.

## 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 ProteomicsAnnotationHubData packages.

## Examples

```
(f <- proteomics(full.names = TRUE))
```

```
library(mzR)
openMSfile(f[1])
```

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