Package 'MSdata'

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Type Package

Title Mass spectrometry data and compiled matrices

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Description A collection of raw mass spectrometry (FIE-MS, FIE-HRMS, LCMS, LC-HRMS) and compiled ``peak mat'' files, which can be used for developing MS processing code and testing / optimising data analysis routines.

License GPL (>= 2)

LazyLoad yes

LazyData yes

ZipData no

R topics documented:

FIEHRMSraw   *Parsed FIE-HRMS mzXML*

Description

Parsed FIE-HRMS mzXML

Usage

```
data(FIEHRMSraw)
```

Format

List object containing 2 elements; `positive` and `negative`, each with 24 sub-elements. The sub-elements of each ionisation mode are the raw parsed output of `mzXML` files using `FIEtools::readFIE`

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Author(s)

Tom Wilson

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pw1HRMS   *Binary (N = 2) High Resolution FIE-MS data set*

Description

Binary (N = 2) High Resolution FIE-MS data set

Usage

```
data(pw1HRMS)
```

Format

List object containing three elements

- pos positive ionisation mode data frame (3079 variables)
- neg negative ionisation mode data frame (1452 variables)
- cls vector of class labels

Author(s)

Tom Wilson

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sin132HRMS   *Large High Resolution FIE-MS data set*

Description

Large High Resolution FIE-MS data set

Usage

```
data(sin132HRMS)
```

Format

List object containing three elements

- pos positive ionisation mode data frame (3079 variables)
- neg negative ionisation mode data frame (1452 variables)
- cls vector of class labels

Author(s)

Tom Wilson

`sin132LTQ` *Large LTQ FIE-MS data set*

Description

Large LTQ FIE-MS data set

Usage

```
data(sin132LTQ)
```

Format

List object containing three elements

- pos positive ionisation mode data frame (742 variables)
- neg negative ionisation mode data frame (688 variables)
- cls vector of class labels

Author(s)

Tom Wilson