

Package ‘iontreeData’

September 23, 2012

Type Package

Title Data provided to show the usage of functions in iontree package

Version 0.99.6

Author Mingshu Cao

Maintainer Mingshu Cao <mingshu.cao@agresearch.co.nz>

Description Raw MS2, MS3 scans from direct infusion mass spectrometry (DIMS) and a demo ion tree database ‘mzDB’ derived from the DIMS data are included. The demo database is used to show the functionalities provided by the ‘iontree’ package, not for the purpose of compound identification by any means.

License GPL-2

biocViews ExperimentData, Metabolomics

LazyLoad yes

R topics documented:

iontreeData-package	1
MS2RAW	2
MS3RAW	3

Index

4

iontreeData-package *Data for iontree package*

Description

There are 3 data sets including raw MS2, MS3 scans ‘MS2RAW’, ‘MS3RAW’ and a SQLite-based ion tree database named ‘mzDB’.

Details

Package:	iontreeData
Type:	Package
Version:	0.99.0
License:	GPL-2
LazyLoad:	yes

Author(s)

Mingshu Cao <mingshu.cao@agresearch.co.nz>

References

Cao M, Koulman A, Johnson LJ, Lane GA and Rasmussen S. 2008. Plant Physiology 146:4

MS2RAW

All the MS2 scans from 4 samples

Description

MS2RAW data from direct infusion mass spectrometry.

Usage

```
data(MS2RAW)
```

Format

see examples

Source

Cao M, Koulman A, Johnson LJ, Lane GA and Rasmussen S. 2008. Plant Physiology 146:4

Examples

```
data(MS2RAW)
length(MS2RAW)
attributes(MS2RAW[[1]])
```

MS3RAW

All the MS3 scans from 4 samples

Description

MS3RAW data from direct infusion mass spectrometry.

Usage

```
data(MS3RAW)
```

Format

see examples

Source

Cao M, Koulman A, Johnson LJ, Lane GA and Rasmussen S. 2008. Plant Physiology 146:4

Examples

```
data(MS3RAW)
```

Index

*Topic **datasets**

 MS2RAW, [2](#)

 MS3RAW, [3](#)

*Topic **package**

 iontreeData-package, [1](#)

 iontreeData (iontreeData-package), [1](#)

 iontreeData-package, [1](#)

 MS2RAW, [2](#)

 MS3RAW, [3](#)