Package 'iontree'

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Type Package

Title Data management and analysis of ion trees from ion-trap mass spectrometry

Version 1.20.0

Depends methods, rJava, RSQLite, XML

Suggests iontreeData

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Description Ion fragmentation provides structural information for metabolite identification. This package provides utility functions to manage and analyse MS2/MS3 fragmentation data from ion trap mass spectrometry. It was designed for high throughput metabolomics data with many biological samples and a large numer of ion trees collected. Tests have been done with data from low-resolution mass spectrometry but could be readily extended to precursor ion based fragmentation data from high resoultion mass spectrometry.

License GPL-2

biocViews Metabolomics, MassSpectrometry

LazyLoad yes

NeedsCompilation no

R topics documented:

`iontree-package` *MSn-iontree: Ion tree management and analysis*

Description

management and analysis of ion fragmentation data

Details

Package:	iontree
Type:	Package
LazyLoad:	yes

This package provides functions to retrieve MSn fragmentation data, build MS2/MS3 ion trees from ion-trap low resoultion mass spectrometry and to create a relational database (SQLite-based) for routine management of ion tree data. Other functions include metrics for MS2 spectral simialrity measurement, iontree plotting and DB operations.

Author(s)

Mingshu Cao
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References

JRAP – a Java library was used for parsing mzXML and mzML
http://sashimi.svn.sourceforge.net/viewvc/sashimi/trunk/jrap/stax/software/

`buildIonTree` *Build ion tree*

Description

build an ion tree derived from the specified m/z and RT ranges in one sample based on ms2 and ms3 raw data, see `saveMSnRaw` and `hasMS2`.

Usage

```
buildIonTree(mzRange = c(340.5, 341.5), rtRange = c(270, 282), ms2, ms3)
```

Arguments

mzRange	mz range
rtRange	rt range
ms2	ms2 data as list
ms3	ms3 data as list

Note

the full time range is used for direct infusion mass spectrometry. For instance, rtRange=c(0, 300) is used for 5-min total elution time.

Author(s)

Mingshu Cao

Examples

```
#mz=867
#mzDelta=0.5
#mzRange=c(mz-mzDelta, mz+mzDelta)
#rtRange=c(1, 600)
#hasMS2(MS2RAW, mzRange=c(mz-mzDelta, mz+mzDelta), rtRange=c(0, 600))

#idx.ms2=1
#ms2=MS2RAW[[idx.ms2]]
#ms3=MS3RAW[[idx.ms2]]

#tree1=buildIonTree(mzRange, rtRange=c(0, 600), ms2, ms3)
#plot(tree1)
```

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createDB *Create a SQLite database*

Description

create a relational database based on a schema defined in this package if argument sql is not specified. There are two tables (experiment and mz) defined to capture necessary information to annotate ions or peaks.

Usage

```
createDB(dbname = "mzDB.db", sql = "mzDBSchema.sql")
```

Arguments

dbname	database name
sql	predefined schema, or a modified definition

Value

A database file saved in the current folder

Author(s)

Mingshu Cao

Examples

```
## Not run:
    createDB(dbname="my.db")

## End(Not run)
```

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distMS2 *Distance metric for MS2 spectral similarity measurement*

Description

distance metric for MS2 spectral comparison. MS2 spectrum is provided as 2-col matrix.

Usage

```
distMS2(a, b, topIon = 20)
```

Arguments

a	MS2 spectrum
b	MS2 spectrum
topIon	the number of the most intense ions used for comparison

Author(s)

Mingshu Cao

References

Cao M, Koulman A, Johnson LJ, Lane GA and Rasmussen S. 2008. Plant Physiology. Vol.146 No.4

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formatSpec *Format mass spec matrix data into a string format, or vice versa*

Description

argument x is a 2-column matrix of mz and intenity, or a string format of mz-internsity paris. Character pair of mz and intensity is separated by semicolon, for example, 150 2345.6; 151 4325.67; .... which is often used to represent a mass spectrum as seen in NIST and MassBank.

Usage

```
formatSpec(x, fromTo = c("mat2str", "str2mat"))
```

Arguments

x	2-col matrix or type of character depends on "fromTo"
fromTo	type of conversion

Author(s)

Mingshu Cao

Examples

```
x="150 2345.6; 151 4325.67;"
formatSpec(x, fromTo="str2mat")
```

---

getMetaInfo *Get metadata information from data file in mzXML*

Description

print out some useful header information, such as instrumentation, ionization, range of mz and RT, and the number of MSn scans etc.

Usage

```
getMetaInfo(filename)
```

Arguments

filename

Author(s)

Mingshu Cao

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getMSnRaw *Get MSn raw data*

Description

query MSn data by the attribute of 'msLevel' and get MSn raw data into a R list. Users may just use function "saveMSnRaw" to retrieve ion tree from a data file and avoid a direct Java function call.

Usage

```
getMSnRaw(msdata, msLevel = 2)
```

Arguments

msdata	msdata is a reference to a Java ArrayList. Obtained by calling getMSData Java function. msdata=.jcall("XCMS", "Ljava/util/ArrayList;","getMSData", filename);
msLevel	msLevel in integer

Value

premz	ancestral precursor ions
rt	retention time
msn.sp	a list of spectrum (m/z, intensity)

Note

MS1 data could be queried by msLevel=1. The return type is still a list but different components (rt, tic, sp).

Author(s)

Mingshu Cao

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hasMS2 *Check which samples have MS2 spectra generated*

Description

check whether MS2 data are available for the ion/peak specified by mzRange and rtRange among samples.

Usage

```
hasMS2(MS2RAW, mzRange = c(1854, 1854.5), rtRange = c(280, 400))
```

Arguments

MS2RAW	MS2 raw data in R binary file, see saveMSnRaw
mzRange	m/z range
rtRange	rt range

Value

return sample index

Author(s)

Mingshu Cao

iontree-class *Class "iontree"*

Description

iontree representation in S4 class

Objects from the Class

Objects can be created by calls of the form `new("iontree", ...)`.

Slots

`mz`: Object of class `"numeric"` peak or ion m/z

`rt`: Object of class `"numeric"` peak or ion RT

`MS2`: Object of class `"matrix"` ms2 spectrum

`MS3`: Object of class `"list"` ms3 spectrum/spectra

Methods

plot `signature(x = "iontree")`: ...

show `signature(object = "iontree")`: ...

Note

To be extended to MSn where n>3

Author(s)

Mingshu Cao

Examples

```
showClass("iontree")
```

metaDataImport *Data entry of meta information*

Description

data entry of table "experiment". Such meta information may include brief description of sample origin, biological treatment, extraction method, chromatography, ionization, polarity, collision energy and those might affect comparative analysis of iontrees. R default data editor was used to help provide necessary informaiton. SQlite database browsers are also freely available for different platforms.

Usage

```
metaDataImport(dbname = "mzDB.db")
```

Arguments

dbname	database name

Note

A known issue: a call to use data editor (fix) might cause access violation, that was occasionally observed.

Author(s)

Mingshu Cao

Examples

```
#to check information just loaded
#db=dbConnect(dbDriver("SQLite"), dbname="mzDB.db")
#dbListTables(db)
#q1=dbSendQuery(db, "SELECT * FROM experiment")
#fetch(q1, n=-1)
#dbClearResult(q1)
#dbDisconnect(db)
```

---

mzImport *Data entry of iontree into mz table*

Description

import iontree object into table "mz" in the database

Usage

```
mzImport(iontree, dbname = "mzDB.db", exp.id)
```

Arguments

iontree	iontree as defined in this package
dbname	database name
exp.id	id in table of experiment

Note

see vignette for an example of batch loading

Author(s)

Mingshu Cao

Examples

```
#to check information just loaded
#db=dbConnect(dbDriver("SQLite"), dbname="mzDB.db")
#dbListTables(db)
#q1=dbSendQuery(db, "SELECT mz, rt, ms2 FROM mz")
#fetch(q1, n=-1)
#dbClearResult(q1)
#dbDisconnect(db)
```

`plot-methods` *Plot iontree*

Description

plot iontree

Methods

`signature(x = "iontree")` plot spectral tree

`plotSpectrum` *Plot a spectrum*

Description

plot a mass spectrum

Usage

```
plotSpectrum(x, y=NULL, top = 20, type = "h", scale100 = FALSE,
    digit.label = 1, col = "black", pos = 0, main = "",
    clickAddLabels = FALSE, ...)
```

Arguments

`x`	m/z
`y`	intensity
`top`	top intense m/z to be labelled
`type`	plot type
`scale100`	in scale of 0-100 if true
`digit.label`	m/z precision to be maintained
`col`	m/z label color
`pos`	m/z label position
`main`	title
`clickAddLabels`	click to add labels
`...`	as in plot

Author(s)

Mingshu Cao

rs2iontree *Convert a data frame into iontree*

Description

Convert resultset, a data frame retrieved from database into a list of iontree objects.

Usage

```
rs2iontree(rs)
```

Arguments

rs	resultset as a data frame

Value

a list of iontrees

Author(s)

Mingshu Cao

saveMSnRaw *Retrieve MS2 and MS3 data and save as R binary in the current folder*

Description

save MS2 and MS3 data for later processing such as ion tree construction. R binary files "MS2RAW.Rdata" and "MS3RAW.Rdata" may be found in the current folder, which can be reloaded.

Usage

```
saveMSnRaw(dataFolder = "D:/Data/Raw")
```

Arguments

dataFolder	current data folder

Author(s)

Mingshu Cao

Examples

```
#saveMSnRaw("D:/Data/Raw")
#load("D:/Data/Raw/MS2RAW.Rdata")
#ls()
```

searchMS2 *Search MS2 spectrum from sqlite database*

Description

search MS2 spetra from the database. Ranking is based on the distance metric that defined by Cao et al. 2008, cosine and Tanimoto similarity.

Usage

```
searchMS2(querySpec, premz, dbname = "mzDB.db", scoreFun = "distMS2", output.record = 5, plot.top =
```

Arguments

querySpec	query spectrum in 2-col matrix
premz	precursor m/z that query spectrum derived from
dbname	database name
scoreFun	score function, 'distMS2','cos' or 'tanimoto'
output.record	the number of records shown in console
plot.top	plot query spectrum and the top-ranked spectrum

Value

return top records

Author(s)

Mingshu Cao

show-methods *Show methods for class iontree*

Description

show methods for class iontree

Methods

signature(object = "iontree") show iontree object

topIons *Retain spectrum with the most intense ions*

Description

Retain the most intense ions in a spectrum and return sorted spectrum in 2-col matrix

Usage

```
topIons(mz, intensity, top)
```

Arguments

mz	m/z
intensity	intensity
top	the number of most intense m/z to be maintained

Value

return a 2-col matrix

Author(s)

Mingshu Cao

Examples

```
#Just sort:
#topIons(mz, intensity, top=length(mz))
```

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