

Package ‘MSEADbi’

March 30, 2021

Title DBI to construct MSEA-related package

Description Interface to construct annotation package for MSEA (MSEA.XXX.pb.db). The program design is same as Bioconductor LRBaseDbi or MeSHDbi pacakge, and the usage is also the same as these packages.

Version 1.0.0

Depends R (>= 4.0)

Imports methods, stats, utils, AnnotationDbi, RSQLite, DBI, Biobase

Suggests RUnit, BiocGenerics, BiocStyle, knitr, testthat (>= 2.1.0)

VignetteBuilder knitr

biocViews Infrastructure

License Artistic-2.0

RoxygenNote 7.1.1

Encoding UTF-8

git_url <https://git.bioconductor.org/packages/MSEADbi>

git_branch RELEASE_3_12

git_last_commit 9f800ce

git_last_commit_date 2020-10-27

Date/Publication 2021-03-29

Author Kozo Nishida [aut, cre] (<<https://orcid.org/0000-0001-8501-7319>>),
Koki Tsuyuzaki [aut] (<<https://orcid.org/0000-0003-3797-2148>>),
Atsushi Fukushima [aut] (<<https://orcid.org/0000-0001-9015-1694>>)

Maintainer Kozo Nishida <kozo.nishida@gmail.com>

R topics documented:

columns	2
dbconn	2
dbfile	3
dbInfo	4
dbschema	4
keys	5
keytypes	5
makeMSEAPackage	6
MSEADb-class	7

mseaListPathwaySubjects	9
mseaNomenclature	9
mseaPackageName	10
mseaVersion	10
select	11
species	12

Index	13
--------------	-----------

columns	<i>A function to return the columns of MSEA that user can retrieve</i>
---------	--

Description

This function returns the columns of MSEA that user can retrieve.

Usage

```
columns(x)
```

Arguments

x MSEADb object such as MSEA.Ath.pb.db

Value

The columns of sqlite database

Author(s)

Kozo Nishida

Examples

```
showMethods("columns")
```

dbconn	<i>A function to return the connection to sqlite3 file</i>
--------	--

Description

This function returns the connection to sqlite file.

Usage

```
dbconn(x)
```

Arguments

x MSEADb object such as MSEA.Ath.pb.db

Value

The database connection to sqlite3 file

Author(s)

Kozo Nishida

Examples

```
showMethods("dbconn")
```

dbfile

A function to return the directory that the sqlite3 file stored

Description

This function returns the directory that the sqlite file stored.

Usage

```
dbfile(x)
```

Arguments

x MSEADb object such as MSEA.Ath.pb.db

Value

The directory path to the sqlite3 file

Author(s)

Kozo Nishida

Examples

```
showMethods("dbfile")
```

dbInfo *A function to return the database information*

Description

This function returns the database information, which is METADATA table in sqlite file.

Usage

```
dbInfo(x)
```

Arguments

x MSEADb object such as MSEA.Ath.pb.db

Value

The information of MSEA.XXX.pb.db package

Author(s)

Kozo Nishida

Examples

```
showMethods("dbInfo")
```

dbschema *A function to return the schema of sqlite-database*

Description

This function returns the schema of sqlite-database.

Usage

```
dbschema(x, file = "", show.indices = FALSE)
```

Arguments

x MSEADb object such as MSEA.Ath.pb.db
file MSEADb file
show.indices MSEADb show.indices

Value

The schema for constructing sqlite database file

Author(s)

Kozo Nishida

Examples

```
showMethods("dbschema")
```

keys	<i>A function defined by AnnotationDbi to return the keys</i>
------	---

Description

This function returns the keys.

Usage

```
keys(x, keytype, ...)
```

Arguments

x	MSEADb object such as MSEA.Ath.pb.db
keytype	MSEADb What kind of key user want to specify
...	MSEADb Other parameter

Value

The keys for using select functions

Author(s)

Kozo Nishida

Examples

```
showMethods("keys")
```

keytypes	<i>A function to return the columns that user can specified in select function</i>
----------	--

Description

This function returns the columns that user can specified in select function.

Usage

```
keytypes(x)
```

Arguments

x	MSEADb object such as MSEA.Ath.pb.db
---	--------------------------------------

Value

The columns that user can specify as key

Author(s)

Kozo Nishida

Examples

```
showMethods("keytypes")
```

makeMSEAPackage	<i>Making MSEADb packages from corresponding table as single data frame.</i>
-----------------	--

Description

makeMSEAPackage is a method that generates a package that will load an appropriate MSEADb object that will in turn point to existing annotation packages.

Usage

```
makeMSEAPackage(
  pkgname,
  data,
  metadata,
  organism,
  version,
  maintainer,
  author,
  destDir,
  license = "Artistic-2.0"
)
```

Arguments

pkgname	What is the desired package name.
data	Data frame contains PathBankID, PathwayName, PathwaySubject, MetaboliteID, MetaboliteName, HMDBID, KEGGID, ChEBIID, DrugBankID, CAS, Formula, IUPAC, SMILES, InChI, and InChIKey
metadata	Data frame contains metadata of the package
organism	The name of the organism this package represents
version	What is the version number for this package?
maintainer	Who is the package maintainer? (must include email to be valid)
author	Who is the creator of this package?
destDir	A path where the package source should be assembled.
license	What is the license (and it's version)

Details

The purpose of this method is to create a special package that will depend on existing annotation packages and which will load a special MSEADb object that will allow proper dispatch of special select methods. These methods will allow the user to easily query across multiple annotation resources via information contained by the MSEADb object. Because the end result will be a package that treats all the data mapped together as a single source, the user is encouraged to take extra care to ensure that the different packages used are from the same build etc.

Value

A special package to load an MSEADb object.

Author(s)

Kozo Nishida

Examples

```
## makeMSEAPackage enable users to construct
## user's own custom MSEA annotation package

## this is test data which means the relationship between
## PathBank pathway IDs of Arabidopsis thaliana
## and its compound DB IDs (e.g., HMDB, CAS, etc...).
tmp <- tempdir()
ath <- system.file("extdata","MSEA.Ath.pb.db_DATA.csv",package="MSEADbi")
meta <- system.file("extdata","MSEA.Ath.pb.db_METADATA.csv",
  package="MSEADbi")
athDf <- read.csv(ath, fileEncoding="utf8")
metaDf <- read.csv(meta)
# We need to avoid DOT from the column names (to query with the names)
names(athDf) <- gsub("\\.", "", names(athDf))
names(metaDf) <- gsub("\\.", "", names(metaDf))

makeMSEAPackage(pkname = "MSEA.Ath.pb.db", data=athDf, metadata=metaDf,
  organism = "Arabidopsis thaliana", version = "0.99.0",
  maintainer = "Kozo Nishida <kozo.nishida@gmail.com>",
  author = "Kozo Nishida",
  destDir = tmp, license = "Artistic-2.0")

mseaPackageDir = paste(tmp,"MSEA.Ath.pb.db", sep="/")
install.packages(mseaPackageDir, repos=NULL, type="source")
```

MSEADb-class

MSEADb objects

Description

MSEADb is the simple class for providing the relationship between PathBank pathway IDs and metabolite IDs contained in the pathway. It provides the database connection and easily accessible with columns, keytypes, keys and select. Some users may use additional functions such as dbconn, dbfile, dbschema, dbInfo, and species for much complex data acquisition.

columns shows which kinds of data can be returned for the MSEADb object.

keytypes allows the user to discover which keytypes can be passed in to select or keys and the keytype argument.

keys returns keys for the database contained in the MSEADb object . This method is already documented in the keys manual page but is mentioned again here because it's usage with select is so intimate. By default it will return the primary keys for the database, but if used with the keytype argument, it will return the keys from that keytype.

select will retrieve the data as a data.frame based on parameters for selected keys, columns, and keytype arguments.

dbconn returns the connection with database in the package.

dbfile returns the absolute path sqlite file is saved.

dbschema returns the database schema.

dbInfo returns the many meta information about the package.

species returns the species name.

Usage

MSEADb

Arguments

MSEADb the MSEADb object. But in practice this will mean an object derived from an MSEADb object such as a MSEA.Ath.pb.db or many other MSEA.XXX.pb.db (XXX means abbreviation of species name).

Value

the MSEADb object

Author(s)

Kozo Nishida

See Also

[dbConnect](#)

Examples

```
ls("package:MSEADbi")
```

`mseaListPathwaySubjects`*A function to return the subject of pathways used in the package*

Description

This function returns the list of pathway subjects used in the package.

Usage

```
mseaListPathwaySubjects(x)
```

Arguments

`x` MSEADb object such as `MSEA.Ath.pb.db`

Value

The list of pathway subjects

Author(s)

Kozo Nishida

Examples

```
showMethods("mseaListPathwaySubjects")
```

`mseaNomenclature`*A function to return the scientific name*

Description

This function returns the scientific name of species used in the package.

Usage

```
mseaNomenclature(x)
```

Arguments

`x` MSEADb object such as `MSEA.Ath.pb.db`

Value

The scientific name of organisms

Author(s)

Kozo Nishida

Examples

```
showMethods("mseaNomenclature")
```

mseaPackageName	<i>A function to return the package name</i>
-----------------	--

Description

This function returns the package name

Usage

```
mseaPackageName(x)
```

Arguments

x MSEADb object such as MSEA.Ath.pb.db

Value

The name of MSEA.XXX.pb.db package

Author(s)

Kozo Nishida

Examples

```
showMethods("mseaPackageName")
```

mseaVersion	<i>A function to return the MSEA data source version of package</i>
-------------	---

Description

This function returns the version of MSEA data source used in the package.

Usage

```
mseaVersion(x)
```

Arguments

x MSEADb object such as MSEA.Ath.pb.db

Value

The version of MSEA database

Author(s)

Kozo Nishida

Examples

```
showMethods("mseaVersion")
```

select

select function defined by AnnotationDbi-class

Description

This function returns the corresponding rows that user specified

Usage

```
select(x, keys, columns, keytype, ...)
```

Arguments

x	MSEADb object such as MSEA.Ath.pb.db
keys	MSEADb keys vector
columns	MSEADb columns the user want to retrieve
keytype	MSEADb What kind of key the user want to specify
...	MSEADb Other parameter

Value

select function defined by AnnotationDbi package

Author(s)

Kozo Nishida

Examples

```
showMethods("select")
```

species

A function to return the name of organism

Description

This function returns the name of organism.

Usage

```
species(object)
```

Arguments

object MSEADb object such as MSEA.Ath.pb.db

Value

The common name of organisms

Author(s)

Kozo Nishida

Examples

```
showMethods("species")
```

Index

class:MSEADb (MSEADb-class), 7
columns, 2
columns,MSEADb-method (columns), 2

dbconn, 2
dbconn,MSEADb-method (dbconn), 2
dbConnect, 8
dbfile, 3
dbfile,MSEADb-method (dbfile), 3
dbInfo, 4
dbInfo,MSEADb-method (dbInfo), 4
dbschema, 4
dbschema,MSEADb-method (dbschema), 4

generic, mseaListPathwaySubjects
 (mseaListPathwaySubjects), 9
generic,columns (columns), 2
generic,dbconn (dbconn), 2
generic,dbfile (dbfile), 3
generic,dbInfo (dbInfo), 4
generic,dbschema (dbschema), 4
generic,keys (keys), 5
generic,keytypes (keytypes), 5
generic,mseaNomenclature
 (mseaNomenclature), 9
generic,mseaPackageName
 (mseaPackageName), 10
generic,mseaVersion (mseaVersion), 10
generic,select (select), 11
generic,species (species), 12

keys, 5
keys,MSEADb-method (keys), 5
keytypes, 5
keytypes,MSEADb-method (keytypes), 5

makeMSEAPackage, 6
MSEADb (MSEADb-class), 7
MSEADb-class, 7
msealistPathwaySubjects, 9
msealistPathwaySubjects,MSEADb-method
 (msealistPathwaySubjects), 9
mseaNomenclature, 9
mseaNomenclature,MSEADb-method
 (mseaNomenclature), 9

mseaPackageName, 10
mseaPackageName,MSEADb-method
 (mseaPackageName), 10
mseaVersion, 10
mseaVersion,MSEADb-method
 (mseaVersion), 10

select, 11
select,MSEADb-method (select), 11
species, 12
species,MSEADb-method (species), 12