Package ‘biodbNci’

February 28, 2024

Title biodbNci, a library for connecting to biodbNci, a library for connecting to the National Cancer Institute (USA) CACTUS Database

Version 1.6.0

Description The biodbNci library is an extension of the biodb framework package. It provides access to biodbNci, a library for connecting to the National Cancer Institute (USA) CACTUS Database. It allows to retrieve entries by their accession number, and run specific web services.

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Imports biodb (>= 1.3.1), R6, Rcpp, chk

LinkingTo Rcpp, testthat

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Collate 'catch-routine-registration.R' 'NciCactusConn.R'

'NciCactusEntry.R' 'RcppExports.R' 'package.R'

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R topics documented:

- biodbNci-package .................. 2
- NciCactusConn ...................... 2
- NciCactusEntry ..................... 5

Index

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biodbNci-package  biodbNci: biodbNci, a library for connecting to biodbNci, a library for connecting to the National Cancer Institute (USA) CACTUS Database

Description

The biodbNci library is an extension of the biodb framework package. It provides access to biodbNci, a library for connecting to the National Cancer Institute (USA) CACTUS Database. It allows to retrieve entries by their accession number, and run specific web services.

Details

See vignette biodbNci:

vignette('biodbNci', package='biodbNci')

Author(s)

Maintainer: Pierrick Roger <pierrick.roger@cea.fr> (ORCID)

See Also

NciCactusConn.

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NciCactusConn  biodbNci, a library for connecting to the National Cancer Institute (USA) CACTUS Database. connector class.

Description

biodbNci, a library for connecting to the National Cancer Institute (USA) CACTUS Database. connector class.

biodbNci, a library for connecting to the National Cancer Institute (USA) CACTUS Database. connector class.
**NciCactusConn**

**Details**

Connector class for biodbNci, a library for connecting to the National Cancer Institute (USA) CACTUS Database.

This class implements a connector for accessing the NCI database, using CACTUS services. See [https://www.cancer.gov/](https://www.cancer.gov/) and [https://cactus.nci.nih.gov/](https://cactus.nci.nih.gov/).

**Super classes**

`biodb::BiodbConnBase -> biodb::BiodbConn -> NciCactusConn`

**Methods**

**Public methods:**

- `NciCactusConn$new()`
- `NciCactusConn$wsChemicalIdentifierResolver()`
- `NciCactusConn$conv()`
- `NciCactusConn$convCasToInchi()`
- `NciCactusConn$convCasToInchikey()`
- `NciCactusConn$clone()`

**Method new():** New instance initializer. Connector classes must not be instantiated directly. Instead, you must use the `createConn()` method of the factory class.

*Usage:*

```r
NciCactusConn$new(...)
```

*Arguments:*

... All parameters are passed to the super class initializer.

*Returns:* Nothing.

**Method wsChemicalIdentifierResolver():** Calls Chemical Identifier Resolver web service. See [https://cactus.nci.nih.gov/chemical/structure_documentation](https://cactus.nci.nih.gov/chemical/structure_documentation) for details.

*Usage:*

```r
NciCactusConn$wsChemicalIdentifierResolver(
  structid,
  repr,
  xml = FALSE,
  retfmt = c("plain", "parsed", "ids", "request")
)
```

*Arguments:*

structid The submitted structure identifier.
repr The wanted representation.
xml A flag for choosing the format returned by the web service between plain text and XML.
retfmt Use to set the format of the returned value. 'plain' will return the raw results from the server, as a character value. 'parsed' will return the parsed results, as an XML object. 'request' will return a BiodbRequest object representing the request as it would have been sent. 'ids' will return a character vector containing the IDs of the matching entries.
Returns: Depending on retfmt parameter.

Method conv(): Calls wsChemicalIdentifierResolver() to convert a list of IDs into another representation.

Usage:
NciCactusConn$conv(ids, repr)

Arguments:
ids A character vector containing IDs.
repr The targeted representation.

Returns: A character vector, the same length as ids, containing the converted IDs. NA values will be set when conversion is not possible.

Method convCasToInchi(): Converts a list of CAS IDs into a list of InChI.

Usage:
NciCactusConn$convCasToInchi(cas)

Arguments:
cas A character vector containing CAS IDs.

Returns: A character vector, the same length as ids, containing InChI values or NA values where conversion was not possible.

Method convCasToInchikey(): Converts a list of CAS IDs into a list of InChI keys.

Usage:
NciCactusConn$convCasToInchikey(cas)

Arguments:
cas A character vector containing CAS IDs.

Returns: A character vector, the same length as ids, containing InChI Key values or NA values where conversion was not possible.

Method clone(): The objects of this class are cloneable with this method.

Usage:
NciCactusConn$clone(deep = FALSE)

Arguments:
dee Whether to make a deep clone.

See Also

BiodbConn.
Examples

# Create an instance with default settings:
mybiodb <- biodb::newInst()

# Get a connector:
conn <- mybiodb$getFactory()$createConn('nci.cactus')

# Use a database extract in order to avoid the downloading of the whole
database.
dbExtract <- system.file('extdata', 'generated', 'cactus_extract.txt.gz',
  package='biodbNci')
conn$setPropValSlot('urls', 'db.gz.url', dbExtract)

# Get an entry
e <- conn$getEntry('749674')

# Terminate instance.
mybiodb$terminate()

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NciCactusEntry

biodbNci, a library for connecting to the National Cancer Institute
(USA) CACTUS Database. entry class.

Description

Entry class for biodbNci, a library for connecting to the National Cancer Institute (USA) CACTUS Database.

Super classes

biodb::BiodbEntry -> biodb::BiodbTxtEntry -> biodb::BiodbSdfEntry -> NciCactusEntry

Methods

Public methods:

• NciCactusEntry$clone()

Method clone(): The objects of this class are cloneable with this method.

Usage:
NciCactusEntry$clone(deep = FALSE)

Arguments:

deep  Whether to make a deep clone.

See Also

BiodbSdfEntry.
Examples

# Create an instance with default settings:
mybiodb <- biodb::newInst()

# Get a connector that inherits from NciCactusConn:
conn <- mybiodb$getFactory()$createConn('nci.cactus')

# Use a database extract in order to avoid the downloading of the whole
# database.
dbExtract <- system.file("extdata", 'generated', "cactus_extract.txt.gz",
                         package="biodbNci")
conn$setPropValSlot('urls', 'db.gz.url', dbExtract)

# Get an entry
e <- conn$getEntry('749674')

# Terminate instance.
mybiodb$terminate()
Index

biodb::BiodbConn, 3
biodb::BiodbConnBase, 3
biodb::BiodbEntry, 5
biodb::BiodbSdfEntry, 5
biodb::BiodbTxtEntry, 5
BiodbConn, 4
biodbNci (biodbNci-package), 2
biodbNci-package, 2
BiodbSdfEntry, 5

NciCactusConn, 2, 2
NciCactusEntry, 5