

Package ‘biodbNci’

April 27, 2025

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

Version 1.12.0

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.

License AGPL-3

biocViews Software, Infrastructure, DataImport

VignetteBuilder knitr

Encoding UTF-8

Depends R (>= 4.1)

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

LinkingTo Rcpp, testthat

Suggests roxygen2, BiocStyle, testthat (>= 2.0.0), devtools, knitr, rmarkdown, covr, lgr

Roxygen list(markdown = TRUE)

RoxygenNote 7.1.2

Collate 'catch-routine-registration.R' 'NciCactusConn.R'
'NciCactusEntry.R' 'RcppExports.R' 'package.R'

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

git_branch RELEASE_3_21

git_last_commit a398ae4

git_last_commit_date 2025-04-15

Repository Bioconductor 3.21

Date/Publication 2025-04-27

Author Pierrick Roger [aut, cre] (ORCID:
<<https://orcid.org/0000-0001-8177-4873>>)

Maintainer Pierrick Roger <pierrick.roger@cea.fr>

Contents

biodbNci-package	2
NciCactusConn	2
NciCactusEntry	5
Index	7

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

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](#).

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

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.

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/> and <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:

```
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 for details.

Usage:

```
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:

deep 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()
```

NciCactusEntry	<i>biodbNci, a library for connecting to the National Cancer Institute (USA) CACTUS Database. entry class.</i>
----------------	--

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](#)