Package 'biodbNci'

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

Version 1.8.0

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

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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)

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See Also

NciCactusConn.

`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.

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` *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()
```

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