Package 'biodbChebi'

October 15, 2023

Title biodbChebi, a library for connecting to the ChEBI Database

Version 1.6.0

Description The biodbChebi library provides access to the ChEBI Database,
using biodb package framework. It allows to retrieve entries by their
accession number. Web services can be accessed for searching the database
by name, mass or other fields.

URL <https://github.com/pkrog/biodbChebi>

BugReports <https://github.com/pkrog/biodbChebi/issues>

biocViews Software, Infrastructure, DataImport

Depends R (>= 4.1)

License AGPL-3

Encoding UTF-8

VignetteBuilder knitr

Suggests BiocStyle, roxygen2, devtools, testthat (>= 2.0.0), knitr,
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RoxygenNote 7.1.2

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R topics documented:

ChebiConn *ChEBI connector class.*

Description

ChEBI connector class.

ChEBI connector class.

Details

This is the connector class for connecting to the ChEBI database through its web services.

Super classes

[biodb::BiodbConnBase](#) -> [biodb::BiodbConn](#) -> ChebiConn

Methods

Public methods:

- [ChebiConn$new()](#)
- [ChebiConn$wsWsdl()](#)
- [ChebiConn$wsGetLiteEntity()](#)
- [ChebiConn$convIdsToChebiIds()](#)
- [ChebiConn$convInchiToChebi()](#)
- [ChebiConn$convCasToChebi()](#)
- [ChebiConn$getWsdl()](#)
- [ChebiConn$getWsdlEnumeration()](#)
- [ChebiConn$getStarsCategories()](#)
- [ChebiConn$getSearchCategories()](#)
- [ChebiConn$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:

ChebiConn$new(...)

Arguments:

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

Returns: Nothing.

Method wsWsdl(): Retrieves the complete WSDL from the web server.

Usage:

ChebiConn$wsWsdl(retfmt = c("plain", "parsed", "request"))

Arguments:

retfmt The return format to use. 'plain' will return the value as it is returned by the server. 'parsed' will return an XML object. 'request' will return a BiodbRequest object representing the request that would have been sent.

Returns: Depending on 'retfmt' value.

Method wsGetLiteEntity(): Calls getLiteEntity web service and returns the XML result. Be careful when searching by mass (search.category='MASS' or 'MONOISOTOPIC MASS'), since the search is made in text mode, thus the number must be exactly written as it is stored in database, eventually padded with 0 in order to have exactly 5 digits after the decimal. An easy solution is to use wildcards to search a mass '410;.718*'. See http //www.ebi.ac.uk/chebi/webServices.do for more details.

Usage:

```
ChebiConn$wsGetLiteEntity(
  search = NULL,
  search.category = "ALL",
  stars = "ALL",
  max.results = 10,
  retfmt = c("plain", "parsed", "request", "ids")
)
```

Arguments:

search The text or pattern to search.

search.category The search category. Call 'getSearchCategories()' to get a full list of search categories.

stars How many starts the returned entities should have. Call 'getStarsCategories() to get a full list of starts categories.'

max.results The maximum of results to return.

retfmt The return format to use. 'plain' will return the results as given by the server, in a string. 'parsed' will return an XML object. 'request' will return a BiodbRequest object representing the request as would have been sent. 'ids' will return a list of matched entity IDs.

Returns: Depending on 'retfmt' value.

Method convIdsToChebiIds(): Converts a list of IDs (InChI, InChI Keys, CAS, ...) into a list of ChEBI IDs. Several ChEBI IDs may be returned for a single ID.

Usage:

```
ChebiConn$convIdsToChebiIds(ids, search.category, simplify = TRUE)
```

Arguments:

ids The identifiers to convert.

search.category The search category. Call 'getSearchCategories()' to get a full list of search categories.

simplify If set to TRUE and only one ChEBI ID has been found for each ID, then a character vector is returned. Otherwise a list of character vectors is returned.

Returns: Depending on the value of simplify.

Method `convInchiToChebi()`: Converts a list of InChI or InChI KEYs into a list of ChEBI IDs. Several ChEBI IDs may be returned for a single InChI or InChI KEY.

Usage:

`ChebiConn$convInchiToChebi(inchi, simplify = TRUE)`

Arguments:

`inchi` The InChI values to convert.

`simplify` If set to TRUE and only one ChEBI ID has been found for each ID, then a character vector is returned. Otherwise a list of character vectors is returned.

Returns: Depending on the value of simplify.

Method `convCasToChebi()`: Converts a list of CAS IDs into a list of ChEBI IDs. Several ChEBI IDs may be returned for a single InChI or InChI KEY.

Usage:

`ChebiConn$convCasToChebi(cas, simplify = TRUE)`

Arguments:

`cas` The CAS IDs to convert.

`simplify` If set to TRUE and only one ChEBI ID has been found for each ID, then a character vector is returned. Otherwise a list of character vectors is returned.

Returns: Depending on the value of simplify.

Method `getWsdl()`: Gets the WSDL as an XML object.

Usage:

`ChebiConn$getWsdl()`

Returns: The ChEBI WSDL as an XML object.

Method `getWsdlEnumeration()`: Extracts a list of values from an enumeration in the WSDL.

Usage:

`ChebiConn$getWsdlEnumeration(name)`

Arguments:

`name` The name of the enumeration for which to retrieve the values.

Returns: A character vector listing the enumerated values.

Method `getStarsCategories()`: Gets the list of allowed stars categories for the getLiteEntity web service.

Usage:

`ChebiConn$getStarsCategories()`

Returns: Returns all the possible stars categories as a character vector.

Method `getSearchCategories()`: Gets the list of allowed search categories for the getLiteEntity web service.

Usage:

`ChebiConn$getSearchCategories()`

Returns: Returns all the possible search categories as a character vector.

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

Usage:

`ChebiConn$clone(deep = FALSE)`

Arguments:

deep Whether to make a deep clone.

Examples

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

# Create a connector
conn <- mybiodb$getFactory()$createConn('chebi')

# Get an entry
e <- conn$getEntry('15440')

# Convert an InChI KEY to a ChEBI identifier
conn$convInchiToChebi('YYGNTYWPHWGJRM-AAJYLUCBSA-N')

# Terminate instance.
mybiodb$terminate()
```

ChebiEntry   *ChEBI entry class.*

Description

This is the entry class for ChEBI database.

Super classes

[biodb::BiodbEntry](#) -> [biodb::BiodbXmlEntry](#) -> ChebiEntry

Methods

Public methods:

- [ChebiEntry$clone()](#)

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

Usage:

`ChebiEntry$clone(deep = FALSE)`

Arguments:

deep Whether to make a deep clone.

Examples

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

# Create a connector to ChEBI
conn <- mybiodb$getFactory()$createConn('chebi')

# Get an entry
e <- conn$getEntry('15440')

# Terminate instance.
mybiodb$terminate()
```

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