

Package ‘biodbChebi’

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Title biodbChebi, a library for connecting to the ChEBI Database

Version 1.0.1

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>

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License AGPL-3

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VignetteBuilder knitr

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ChebiConn	<i>ChEBI connector class.</i>
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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 stars the returned entities should have. Call `'getStarsCategories()'` to get a full list of stars 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 getWsd1(): Gets the WSDL as an XML object.

Usage:

```
ChebiConn$getWsd1()
```

Returns: The ChEBI WSDL as an XML object.

Method getWsd1Enumeration(): Extracts a list of values from an enumeration in the WSDL.

Usage:

```
ChebiConn$getWsd1Enumeration(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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