# Package 'biodbKegg'

March 25, 2024

**Title** biodbKegg, a library for connecting to the KEGG Database

Version 1.8.0

Description The biodbKegg library is an extension of the biodb framework package that provides access to the KEGG databases Compound, Enzyme, Genes, Module, Orthology and Reaction. It allows to retrieve entries by their accession numbers. Web services like ``find", ``list" and ``findExactMass" are also available. Some functions for navigating along the pathways have also been implemented.

URL https://github.com/pkrog/biodbKegg

BugReports https://github.com/pkrog/biodbKegg/issues

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'KeggEntry.R' 'KeggCompoundEntry.R' 'KeggEnzymeConn.R'

'KeggEnzymeEntry.R' 'KeggGenesConn.R' 'KeggGenesEntry.R'

'KeggGlycanConn.R' 'KeggGlycanEntry.R' 'KeggModuleConn.R'

'KeggModuleEntry.R' 'KeggOrthologyConn.R'

'KeggOrthologyEntry.R' 'KeggPathwayConn.R' 'KeggPathwayEntry.R'

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

Maintainer Pierrick Roger pierrick.roger@cea.fr>

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KeggCircle

A class for representing a circle.

### Description

A class for representing a circle.

A class for representing a circle.

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### **Details**

This class represents a rectangle, used for graphical representation. It is used by KeggPathway-Conn::extractPathwayMapShapes() method.

Arguments to the constructor are:

x: X coordinate of center.

y: Y coordinate of center.

r: Radius.

### Super class

```
biodbKegg::KeggShape -> KeggCircle
```

#### Methods

#### **Public methods:**

```
• KeggCircle$new()
```

- KeggCircle\$getX()
- KeggCircle\$getY()
- KeggCircle\$getRadius()
- KeggCircle\$clone()

```
Method new(): Initialize new instance.
```

```
Usage:
```

```
KeggCircle$new(x, y, r, ...)
```

Arguments:

- x Abscissa of the circle's center.
- y Ordinate of the circle's center.
- r Radius of the circle.
- ... Additional parameters are passed to super class' initializer.

Returns: Nothing.

### **Method** getX(): Get the X coordinate.

Usage:

KeggCircle\$getX()

Returns: The X coordinate.

### **Method** getY(): Get the Y coordinate.

Usage:

KeggCircle\$getY()

Returns: The Y coordinate.

### Method getRadius(): Get the radius.

Usage:

```
KeggCircle$getRadius()
Returns: The radius.

Method clone(): The objects of this class are cloneable with this method.
Usage:
KeggCircle$clone(deep = FALSE)
Arguments:
deep Whether to make a deep clone.
```

#### See Also

KeggShape, KeggRect.

#### **Examples**

```
# Create an instance
c1 <- KeggCircle$new(x=12, y=5, r=3)

# Since it inherits from KeggShape, a color and a label can be set
c2 <- KeggCircle$new(x=12, y=5, r=3, color='blue', label='Circle 2')

# Getting center
c1$getX()
c1$getY()

# Getting radius
c1#getRadius()

# Draw a circle on the current image
c1$draw()</pre>
```

 ${\sf KeggCompoundConn}$ 

The connector class to KEGG Compound database.

### **Description**

The connector class to KEGG Compound database.

The connector class to KEGG Compound database.

#### **Details**

This is a concrete connector class. It must never be instantiated directly, but instead be instantiated through the factory BiodbFactory. Only specific methods are described here. See super classes for the description of inherited methods.

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### Super classes

```
biodb::BiodbConnBase->biodb::BiodbConn->biodbKegg::KeggConn->KeggCompoundConn
```

#### Methods

#### **Public methods:**

- KeggCompoundConn\$new()
- KeggCompoundConn\$wsFindExactMass()
- KeggCompoundConn\$wsFindMolecularWeight()
- KeggCompoundConn\$getPathwayIdsPerCompound()
- KeggCompoundConn\$getModuleIdsPerCompound()
- KeggCompoundConn\$getPathwayIds()
- KeggCompoundConn\$addInfo()
- KeggCompoundConn\$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:KeggCompoundConn$new(...)Arguments:... All parameters are passed to the super class initializer.Returns: Nothing.
```

**Method** wsFindExactMass(): Searches for entries by mass. You must either provide a single mass through 'mass' parameter or provide a range through 'mass.min' and 'mass.max'.

```
KeggCompoundConn$wsFindExactMass(
    mass = NULL,
    mass.min = NULL,
    mass.max = NULL,
    ...
)

Arguments:
mass Single mass.
mass.min Minimal mass.
mass.max Maximal mass.
... parameters passed to KeggConn::wsFind().
See http://www.kegg.jp/kegg/docs/keggapi.html for details.

Returns: wsFind().
```

**Method** wsFindMolecularWeight(): Searches for entries by molecular mass. You must either provide a single mass through 'mass' parameter or provide a range through 'mass.min' and 'mass.max'. See http://www.kegg.jp/kegg/docs/keggapi.html for details.

Usage:

KeggCompoundConn

```
KeggCompoundConn$wsFindMolecularWeight(
  mass = NULL,
  mass.min = NULL,
  mass.max = NULL,
    ...
)
Arguments:
mass Single mass.
mass.min Minimal mass.
mass.max Maximal mass.
... Parameters passed to KeggConn::wsFind().
Returns: wsFind().
```

**Method** getPathwayIdsPerCompound(): Gets organism pathways for each compound. This method retrieves for each compound the KEGG pathways of the organism in which the compound is involved.

Usage:

KeggCompoundConn\$getPathwayIdsPerCompound(id, org, limit = 3)

Arguments:

id A character vector of KEGG Compound IDs.

org The organism in which to search for pathways, as a KEGG organism code (3-4 letters code, like 'hsa', 'mmu', ...). See https://www.genome.jp/kegg/catalog/org\_list.html for a complete list of KEGG organism codes.

limit The maximum number of modules IDs to retrieve for each compound. Set to 0 to disable.

Returns: A named list of KEGG pathway ID vectors, where the names of the list are the compound IDs."

**Method** getModuleIdsPerCompound(): Gets organism modules for each compound. This method retrieves for each compound the KEGG modules of the organism in which the compound is involved.

Usage:

KeggCompoundConn\$getModuleIdsPerCompound(id, org, limit = 3)

Arguments:

id A character vector of KEGG Compound IDs.

org The organism in which to search for modules, as a KEGG organism code (3-4 letters code, like 'hsa', 'mmu', ...). See https://www.genome.jp/kegg/catalog/org\_list.html for a complete list of KEGG organism codes.

limit The maximum number of modules IDs to retrieve for each compound. Set to 0 to disable.

*Returns:* A named list of KEGG module ID vectors, where the names of the list are the compound IDs."

**Method** getPathwayIds(): Gets organism pathways. This method retrieves KEGG pathways of the specified organism in which the compounds are involved.

Usage:

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KeggCompoundConn\$getPathwayIds(id, org)

Arguments:

id A character vector of KEGG Compound IDs.

org The organism in which to search for pathways, as a KEGG organism code (3-4 letters code, like 'hsa', 'mmu', ...). See https://www.genome.jp/kegg/catalog/org\_list.html for a complete list of KEGG organism codes.

Returns: A vector of KEGG pathway IDs.

**Method** addInfo(): Add informations (as new column appended to the end) to an existing data frame containing a column of KEGG Compound IDs.

Usage:

```
KeggCompoundConn$addInfo(x, id.col, org, limit = 3, prefix = "")
```

Arguments

- x A data frame containing at least one column with Biodb entry IDs identified by the parameter 'id.col'.
- id.col The name of the column containing IDs inside the input data frame.
- org The organism in which to search for pathways, as a KEGG organism code (3-4 letters code, like 'hsa', 'mmu', ...). See https://www.genome.jp/kegg/catalog/org\_list.html for a complete list of KEGG organism codes.
- limit This is the maximum number of values obtained for each ID, for every column added, in case multiple values are obtained. Set to 0 to get all values.
- prefix Insert a prefix at the start of name of all new columns.

Returns: A data frame containing 'x' and new columns appended with KEGG identifiers and data.

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

Usage.

KeggCompoundConn\$clone(deep = FALSE)

Arguments:

deep Whether to make a deep clone.

#### See Also

KeggConn, KeggPathwayConn.

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

# Create a connector to KEGG Compound
conn <- mybiodb$getFactory()$createConn('kegg.compound')

# Search for compounds by exact mass
conn$wsFindExactMass(mass=174.05, retfmt='parsed')</pre>
```

```
# Search for compounds by molecular weight
conn$wsFindMolecularWeight(mass=300, retfmt='parsed')
# Get pathway IDs related to compounds
pathway.ids=conn$getPathwayIds(c('C02648', 'C06144'), org='mmu')
# Terminate instance.
mybiodb$terminate()
```

KeggCompoundEntry

KEGG Compound entry class.

### Description

This is the entry class for the KEGG Compound database.

### Super classes

```
biodb::BiodbEntry->biodb::BiodbTxtEntry->biodbKegg::KeggEntry->KeggCompoundEntry
```

#### Methods

### **Public methods:**

• KeggCompoundEntry\$clone()

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

Usage:

KeggCompoundEntry\$clone(deep = FALSE)

Arguments:

deep Whether to make a deep clone.

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

# Create a connector
conn <- mybiodb$getFactory()$createConn('kegg.compound')

# Get an entry
e <- conn$getEntry('C00133')

# Terminate instance.
mybiodb$terminate()</pre>
```

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KeggConn

The connector abstract class to KEGG databases.

#### **Description**

The connector abstract class to KEGG databases.

The connector abstract class to KEGG databases.

#### **Details**

This is the mother class of all KEGG connectors. It defines code common to all KEGG connectors.

The constructor accepts the following arguments:

db.name: The database name as defined in http://www.kegg.jp/kegg/docs/keggapi.html.

db.abbrev: The database abbreviated name, as defined in http://www.kegg.jp/kegg/docs/keggapi.html.

### Super classes

```
biodb::BiodbConnBase -> biodb::BiodbConn -> KeggConn
```

#### Methods

#### **Public methods:**

- KeggConn\$new()
- KeggConn\$wsList()
- KeggConn\$wsFind()
- KeggConn\$clone()

**Method** new(): New instance initializer. Connector classes must not be instantiated directly. Instead, you must use the createConn() method of the factory class. The parameters of this function are for the use of subclasses.

```
Usage:
KeggConn$new(
  db.name = NA_character_,
  db.abbrev = NA_character_,
  accession.prefix = NA_character_,
  ...
)
Arguments:
```

db.name The database name as defined in www.kegg.jp/kegg/docs/keggapi.html.

db. abbrev The database abbreviation as defined in www.kegg.jp/kegg/docs/keggapi.html. accession.prefix The prefix used for accession identifiers.

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

Returns: Nothing.

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**Method** wsList(): Gets the full list of entry IDs. See

```
KeggConn$wsList(retfmt = c("plain", "request", "ids"))
 Arguments:
 retfmt Use to set the format of the returned value. 'plain' will return the raw result from the
     server, as a character value. 'request' will return the request as it would have been sent, as
     a BiodbRequest object. 'ids' will return a character vector containing entry IDs.
 http://www.kegg.jp/kegg/docs/keggapi.html for details.
 Returns: Depending on 'retfmt'.
Method wsFind(): Searches for entries. See http://www.kegg.jp/kegg/docs/keggapi.html for
details.
 Usage:
 KeggConn$wsFind(
    query,
    option = c("NONE", "formula", "exact_mass", "mol_weight", "nop"),
    retfmt = c("plain", "request", "parsed", "ids", "ids.no.prefix")
 )
 Arguments:
 query The query to send to the database web service. When searching by mass (i.e. 'option'
     parameter set to either 'exact mass' or 'mol weight'), this query field must be set to either
     an exact (i.e. 174.05) or a range (i.e. '250-260').
 option Set this parameter to 'NONE' for querying on fields 'ENTRY', 'NAME', 'DESCRIP-
     TION', 'COMPOSITION', 'DEFINITION' and 'ORTHOLOGY'. See http://www.kegg.jp/kegg/docs/keggapi.html
     for an exact list of fields that are searched for each database, and also for other possible val-
     ues of this 'option' paramater.
 retfmt Use to set the format of the returned value. 'plain' will return the raw result from the
     server, as a character value. 'request' will return the request as it would have been sent, as a
     BiodbRequest object. 'parsed' will return a data frame. 'ids' will return a character vector
     containing the IDs of the matching entries.
 Returns: Depending on 'retfmt'.
Method clone(): The objects of this class are cloneable with this method.
 KeggConn$clone(deep = FALSE)
 Arguments:
 deep Whether to make a deep clone.
```

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

# Create a connector to a KEGG database
conn <- mybiodb$getFactory()$createConn('kegg.compound')</pre>
```

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```
# Search for an entry
conn$wsFind('NADPH', retfmt='parsed')
# Terminate instance.
mybiodb$terminate()
```

KeggEntry

KEGG entry abstract class.

### **Description**

This is the abstract entry class for all KEGG entry classes.

### Super classes

```
biodb::BiodbEntry -> biodb::BiodbTxtEntry -> KeggEntry
```

#### Methods

### **Public methods:**

• KeggEntry\$clone()

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

```
Usage:
```

```
KeggEntry$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

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

# Create a connector
conn <- mybiodb$getFactory()$createConn('kegg.compound')

# Get an entry
e <- conn$getEntry('C00133')

# Terminate instance.
mybiodb$terminate()</pre>
```

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KeggEnzymeConn

The connector class to KEGG Enzyme database.

#### **Description**

The connector class to KEGG Enzyme database.

The connector class to KEGG Enzyme database.

#### **Details**

This is a concrete connector class. It must never be instantiated directly, but instead be instantiated through the factory BiodbFactory. Only specific methods are described here. See super classes for the description of inherited methods.

#### Super classes

```
biodb::BiodbConnBase -> biodb::BiodbConn -> biodbKegg::KeggConn -> KeggEnzymeConn
```

#### Methods

#### **Public methods:**

- KeggEnzymeConn\$new()
- KeggEnzymeConn\$getPathwayIds()
- KeggEnzymeConn\$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:
```

KeggEnzymeConn\$new(...)

Arguments:

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

Returns: Nothing.

**Method** getPathwayIds(): Gets organism pathways. This method retrieves KEGG pathways of the specified organism in which the enzymes are involved.

Usage:

KeggEnzymeConn\$getPathwayIds(id, org)

Arguments:

id A character vector of KEGG Compound IDs.

org The organism in which to search for pathways, as a KEGG organism code (3-4 letters code, like 'hsa', 'mmu', ...). See https://www.genome.jp/kegg/catalog/org\_list.html for a complete list of KEGG organism codes.

Returns: A vector of KEGG pathway IDs.

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

Usage.

KeggEnzymeConn\$clone(deep = FALSE)

Arguments:

deep Whether to make a deep clone.

#### See Also

KeggConn.

### **Examples**

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

# Get connector
conn <- mybiodb$getFactory()$createConn('kegg.enzyme')

# Get pathway IDs related to enzymes
pathway.ids=conn$getPathwayIds(c('1.2.1.3', '3.7.1.3'), org='mmu')

# Terminate instance.
mybiodb$terminate()</pre>
```

KeggEnzymeEntry

KEGG Enzyme entry class.

### Description

This is the entry class for the KEGG Enzyme class.

### Super classes

```
biodb::BiodbEntry->biodb::BiodbTxtEntry->biodbKegg::KeggEntry->KeggEnzymeEntry
```

#### Methods

### **Public methods:**

• KeggEnzymeEntry\$clone()

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

Usage:

```
KeggEnzymeEntry$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

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#### **Examples**

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

# Create a connector
conn <- mybiodb$getFactory()$createConn('kegg.enzyme')

# Get an entry
e <- conn$getEntry('1.1.1.54')

# Terminate instance.
mybiodb$terminate()</pre>
```

KeggGenesConn

The connector class to KEGG Pathway database.

### **Description**

The connector class to KEGG Pathway database.

The connector class to KEGG Pathway database.

#### **Details**

This is a concrete connector class. It must never be instantiated directly, but instead be instantiated through the factory BiodbFactory. Only specific methods are described here. See super classes for the description of inherited methods.

### Super classes

```
biodb::BiodbConnBase -> biodb::BiodbConn -> biodbKegg::KeggConn -> KeggGenesConn
```

#### Methods

#### **Public methods:**

- KeggGenesConn\$new()
- KeggGenesConn\$getPathwayIdsPerGene()
- KeggGenesConn\$getPathwayIds()
- KeggGenesConn\$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:
KeggGenesConn$new(...)
Arguments:
... All parameters are passed to the super class initializer.
```

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Returns: Nothing.

**Method** getPathwayIdsPerGene(): Gets organism pathways for each gene. This method retrieves for each gene the KEGG pathways of the organism in which the gene is involved.

Usage:

KeggGenesConn\$getPathwayIdsPerGene(id, org, limit = 3)

Arguments:

id A character vector of KEGG Gene IDs.

org The organism in which to search for pathways, as a KEGG organism code (3-4 letters code, like 'hsa', 'mmu', ...). See https://www.genome.jp/kegg/catalog/org\_list.html for a complete list of KEGG organism codes.

limit The maximum number of modules IDs to retrieve for each gene. Set to 0 to disable.

*Returns:* A named list of KEGG pathway ID vectors, where the names of the list are the gene IDs."

**Method** getPathwayIds(): Gets organism pathways. This method retrieves KEGG pathways of the specified organism in which the genes are involved.

Usage:

KeggGenesConn\$getPathwayIds(id, org)

Arguments:

id A character vector of KEGG Genes IDs.

org The organism in which to search for pathways, as a KEGG organism code (3-4 letters code, like 'hsa', 'mmu', ...). See https://www.genome.jp/kegg/catalog/org\_list.html for a complete list of KEGG organism codes.

Returns: A vector of KEGG pathway IDs.

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

Usage:

KeggGenesConn\$clone(deep = FALSE)

Arguments:

deep Whether to make a deep clone.

### See Also

KeggConn.

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

# Create a connector
conn <- mybiodb$getFactory()$createConn('kegg.genes')

# Get an entry
e <- conn$getEntry('mmu:14635')</pre>
```

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

KeggGenesEntry

KEGG Genes entry class.

### Description

This is the entry class for the KEGG Genes database.

### Super classes

```
biodb::BiodbEntry -> biodb::BiodbTxtEntry -> biodbKegg::KeggEntry -> KeggGenesEntry
```

### Methods

### **Public methods:**

• KeggGenesEntry\$clone()

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

Usage:

KeggGenesEntry\$clone(deep = FALSE)

Arguments:

deep Whether to make a deep clone.

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

# Create a connector
conn <- mybiodb$getFactory()$createConn('kegg.genes')

# Get an entry
e <- conn$getEntry('mmu:14635')

# Terminate instance.
mybiodb$terminate()</pre>
```

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VESSOT	vcanconn

The connector class to KEGG Glycan database.

### **Description**

The connector class to KEGG Glycan database.

The connector class to KEGG Glycan database.

#### **Details**

This is a concrete connector class. It must never be instantiated directly, but instead be instantiated through the factory BiodbFactory. Only specific methods are described here. See super classes for the description of inherited methods.

### Super classes

```
biodb::BiodbConnBase -> biodb::BiodbConn -> biodbKegg::KeggConn -> KeggGlycanConn
```

#### Methods

#### **Public methods:**

- KeggGlycanConn\$new()
- KeggGlycanConn\$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:
KeggGlycanConn$new(...)
Arguments:
... All parameters are passed to the super class initializer.
Returns: Nothing.

Method clone(): The objects of this class are cloneable with this method.
Usage:
KeggGlycanConn$clone(deep = FALSE)
Arguments:
deep Whether to make a deep clone.
```

#### See Also

KeggConn.

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#### **Examples**

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

# Create a connector to KEGG Glycan
conn <- mybiodb$getFactory()$createConn('kegg.glycan')

# Terminate instance.
mybiodb$terminate()</pre>
```

KeggGlycanEntry

KEGG Glycan entry class.

### Description

This is the entry class for the KEGG Glycan database.

### Super classes

```
biodb::BiodbEntry -> biodb::BiodbTxtEntry -> biodbKegg::KeggEntry -> KeggGlycanEntry
```

#### Methods

#### **Public methods:**

• KeggGlycanEntry\$clone()

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

```
Usage:
KeggGlycanEntry$clone(deep = FALSE)
Arguments:
deep Whether to make a deep clone.
```

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

# Create a connector
conn <- mybiodb$getFactory()$createConn('kegg.glycan')

# Get an entry
e <- conn$getEntry('G00018')

# Terminate instance.
mybiodb$terminate()</pre>
```

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The connector class to KEGG Pathway database.

### **Description**

The connector class to KEGG Pathway database.

The connector class to KEGG Pathway database.

#### **Details**

This is a concrete connector class. It must never be instantiated directly, but instead be instantiated through the factory BiodbFactory. Only specific methods are described here. See super classes for the description of inherited methods.

### Super classes

```
biodb::BiodbConnBase -> biodb::BiodbConn -> biodbKegg::KeggConn -> KeggModuleConn
```

#### Methods

#### **Public methods:**

- KeggModuleConn\$new()
- KeggModuleConn\$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:
KeggModuleConn$new(...)
Arguments:
... All parameters are passed to the super class initializer.
Returns: Nothing.

Method clone(): The objects of this class are cloneable with this method.
Usage:
KeggModuleConn$clone(deep = FALSE)
Arguments:
deep Whether to make a deep clone.
```

#### See Also

KeggConn.

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#### **Examples**

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

# Create a connector
conn <- mybiodb$getFactory()$createConn('kegg.module')

# Get an entry
e <- conn$getEntry('M00009')

# Terminate instance.
mybiodb$terminate()</pre>
```

KeggModuleEntry

KEGG Module entry class.

#### **Description**

This is the entry class for KEGG Module database

#### Super classes

```
biodb::BiodbEntry->biodb::BiodbTxtEntry->biodbKegg::KeggEntry->KeggModuleEntry
```

### Methods

#### **Public methods:**

• KeggModuleEntry\$clone()

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

```
Usage:
```

KeggModuleEntry\$clone(deep = FALSE)

Arguments:

deep Whether to make a deep clone.

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

# Create a connector
conn <- mybiodb$getFactory()$createConn('kegg.module')

# Get an entry
e <- conn$getEntry('M00009')

# Terminate instance.
mybiodb$terminate()</pre>
```

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KeggOrthologyConn

The connector class to KEGG Orthology database.

### Description

The connector class to KEGG Orthology database.

The connector class to KEGG Orthology database.

#### **Details**

This is a concrete connector class. It must never be instantiated directly, but instead be instantiated through the factory BiodbFactory. Only specific methods are described here. See super classes for the description of inherited methods.

### Super classes

```
biodb::BiodbConnBase->biodb::BiodbConn->biodbKegg::KeggConn->KeggOrthologyConn
```

#### Methods

#### **Public methods:**

- KeggOrthologyConn\$new()
- KeggOrthologyConn\$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:
KeggOrthologyConn$new(...)
Arguments:
... All parameters are passed to the super class initializer.
Returns: Nothing.

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

KeggOrthologyConn\$clone(deep = FALSE)

deep Whether to make a deep clone.

See Also

KeggConn.

Arguments:

#### **Examples**

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

# Create a connector
conn <- mybiodb$getFactory()$createConn('kegg.orthology')

# Get an entry
e <- conn$getEntry('K12668')

# Terminate instance.
mybiodb$terminate()</pre>
```

KeggOrthologyEntry

KEGG Orthology entry class.

#### **Description**

This is the class entry for KEGG Orthology database.

### Super classes

```
biodb::BiodbEntry->biodb::BiodbTxtEntry->biodbKegg::KeggEntry->KeggOrthologyEntry
```

### Methods

#### **Public methods:**

• KeggOrthologyEntry\$clone()

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

```
Usage:
```

KeggOrthologyEntry\$clone(deep = FALSE)

Arguments:

deep Whether to make a deep clone.

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

# Create a connector
conn <- mybiodb$getFactory()$createConn('kegg.orthology')

# Get an entry
e <- conn$getEntry('K12668')

# Terminate instance.
mybiodb$terminate()</pre>
```

KeggPathwayConn 23

KeggPathwayConn

The connector class to KEGG Pathway database.

#### **Description**

The connector class to KEGG Pathway database.

The connector class to KEGG Pathway database.

#### **Details**

This is a concrete connector class. It must never be instantiated directly, but instead be instantiated through the factory BiodbFactory. Only specific methods are described here. See super classes for the description of inherited methods.

#### Super classes

```
biodb::BiodbConnBase -> biodb::BiodbConn -> biodbKegg::KeggConn -> KeggPathwayConn
```

#### Methods

#### **Public methods:**

- KeggPathwayConn\$new()
- KeggPathwayConn\$getReactions()
- KeggPathwayConn\$convertToOrgPathways()
- KeggPathwayConn\$buildPathwayGraph()
- KeggPathwayConn\$getPathwayIgraph()
- KeggPathwayConn\$getDecoratedGraphPicture()
- KeggPathwayConn\$extractPathwayMapShapes()
- KeggPathwayConn\$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:
```

KeggPathwayConn\$new(...)

Arguments:

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

Returns: Nothing.

**Method** getReactions(): Retrieves all reactions part of a KEGG pathway. Connects to KEGG databases, and walk through all pathways submitted, and their modules, to find all reactions they are composed of.

```
Usage:
```

```
KeggPathwayConn$getReactions(id, drop = TRUE)
```

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Arguments:

id A character vector of entry IDs.

drop If set to TRUE, returns a single KEGG reaction object instead of a list, if the list contains only one element.

Returns: A list of KEGG reaction objects.

**Method** convertToOrgPathways(): Takes a list of pathways IDs and converts them to the specified organism, filtering out the ones that do not exist in KEGG.

Usage:

KeggPathwayConn\$convertToOrgPathways(id, org)

Arguments:

id A character vector of entry IDs.

org The organism in which to search for pathways, as a KEGG organism code (3-4 letters code, like 'hsa', 'mmu', ...). See https://www.genome.jp/kegg/catalog/org\_list.html for a complete list of KEGG organism codes.

Returns: A character vector, the same length as 'id', containing the converted IDs.

**Method** buildPathwayGraph(): Builds a pathway graph in the form of two tables of vertices and edges, using KEGG database.

Usage:

KeggPathwayConn\$buildPathwayGraph(id, directed = FALSE, drop = TRUE)

Arguments:

id A character vector of KEGG pathway entry IDs.

directed If set to TRUE, use available direction information to create directed edges, duplicating if necessary the vertices.

drop If set to TRUE and the output list contains only one element, then the returned value is a single list of two data frames.

*Returns:* A named list whose names are the pathway IDs, and values are lists containing two data frames named vertices and edges.

**Method** getPathwayIgraph(): Builds a pathway graph, as an igraph object, using KEGG database.

Usage:

KeggPathwayConn\$getPathwayIgraph(id, directed = FALSE, drop = TRUE)

Arguments.

id A character vector of KEGG pathway entry IDs.

directed If set to TRUE, use available direction information to create directed edges, duplicating if necessary the vertices.

drop If set to TRUE and the output list contains only one element, then the returned value is a single igraph object.

Returns: A list of igraph objects, or an empty list if the igraph library is not available.

**Method** getDecoratedGraphPicture(): Create a pathway graph picture, with some of its elements colorized.

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```
Usage:
```

KeggPathwayConn\$getDecoratedGraphPicture(id, color2ids)

Arguments:

id A KEGG pathway ID.

color2ids A named list defining colors for entry IDs that are present on the graph. The names of the list are standard color names. The values are character vector of entry IDs.

Returns: An image object or NULL if the package magick is not available.

**Method** extractPathwayMapShapes(): Extracts shapes from a pathway map image.

Usage:

KeggPathwayConn\$extractPathwayMapShapes(id, color2ids)

Arguments:

id A KEGG pathway ID.

color2ids A named list defining colors for entry IDs that are present on the graph. The names of the list are standard color names. The values are character vector of entry IDs.

Returns: A list of BiodbShape objects.

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

Usage:

KeggPathwayConn\$clone(deep = FALSE)

Arguments:

deep Whether to make a deep clone.

#### See Also

KeggConn.

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

# Get connector
conn=mybiodb$getFactory()$createConn('kegg.pathway')

# Retrieve all reactions related to a mouse pathway:
reactions=conn$getReactions('mmu00260')

# Get a pathway graph
graph=conn$buildPathwayGraph('mmu00260')

# Terminate instance.
mybiodb$terminate()</pre>
```

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KeggPathwayEntry

KEGG Pathway entry class.

### Description

This is the class entry for KEGG Pathway database.

### Super classes

```
biodb::BiodbEntry->biodb::BiodbTxtEntry->biodbKegg::KeggEntry->KeggPathwayEntry
```

#### Methods

#### **Public methods:**

• KeggPathwayEntry\$clone()

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

```
Usage:
```

KeggPathwayEntry\$clone(deep = FALSE)

Arguments:

deep Whether to make a deep clone.

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

# Create a connector
conn <- mybiodb$getFactory()$createConn('kegg.pathway')

# Get an entry
e <- conn$getEntry('map00053')

# Terminate instance.
mybiodb$terminate()</pre>
```

KeggReactionConn 27

KeggReactionConn

The connector class to KEGG Reaction database.

### Description

The connector class to KEGG Reaction database.

The connector class to KEGG Reaction database.

#### **Details**

This is a concrete connector class. It must never be instantiated directly, but instead be instantiated through the factory BiodbFactory. Only specific methods are described here. See super classes for the description of inherited methods.

### Super classes

```
biodb::BiodbConnBase -> biodb::BiodbConn -> biodbKegg::KeggConn -> KeggReactionConn
```

#### Methods

#### **Public methods:**

- KeggReactionConn\$new()
- KeggReactionConn\$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:
KeggReactionConn$new(...)
Arguments:
... All parameters are passed to the super class initializer.
Returns: Nothing.

Method clone(): The objects of this class are cloneable with this method.
Usage:
KeggReactionConn$clone(deep = FALSE)
Arguments:
deep Whether to make a deep clone.
```

#### See Also

KeggConn.

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#### **Examples**

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

# Create a connector
conn <- mybiodb$getFactory()$createConn('kegg.reaction')

# Get an entry
e <- conn$getEntry('R00105')

# Terminate instance.
mybiodb$terminate()</pre>
```

KeggReactionEntry

KEGG Reaction entry class.

#### **Description**

This is the entry class for KEGG Reation database.

#### Super classes

```
biodb::BiodbEntry->biodb::BiodbTxtEntry->biodbKegg::KeggEntry->KeggReactionEntry
```

### Methods

#### **Public methods:**

• KeggReactionEntry\$clone()

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

```
Usage:
```

KeggReactionEntry\$clone(deep = FALSE)

Arguments:

deep Whether to make a deep clone.

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

# Create a connector
conn <- mybiodb$getFactory()$createConn('kegg.reaction')

# Get an entry
e <- conn$getEntry('R00105')

# Terminate instance.
mybiodb$terminate()</pre>
```

KeggRect 29

KeggRect

A class for representing a rectangle.

### **Description**

A class for representing a rectangle.

A class for representing a rectangle.

#### **Details**

This class represents a rectangle, used for graphical representation.

Arguments to the constructor are:

left: Coordinate of left border.

right: Coordinate of right border.

top: Coordinate of top border.

bottom: Coordinate of bottom border.

#### Super class

```
biodbKegg::KeggShape -> KeggRect
```

#### Methods

### **Public methods:**

- KeggRect\$new()
- KeggRect\$clone()

```
Method new(): Initialize new instance.
```

```
Usage:
```

```
KeggRect$new(left, top, bottom, right, ...)
```

Arguments:

left Coordinate of rectangle's left side.

top Coordinate of rectangle's top side.

bottom Coordinate of rectangle's bottom side.

right Coordinate of rectangle's right side.

... Additional parameters are passed to super class' initializer.

Returns: Nothing.

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

Usage:

```
KeggRect$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

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#### See Also

```
KeggShape, KeggCircle.
```

#### **Examples**

```
# Create a rectangle instance
r <- KeggRect$new(left=10, top=10, bottom=20, right=30, color='yellow')
# Draw a rectangle on current image
r$draw()</pre>
```

KeggShape

A class for representing a shape.

### Description

A class for representing a shape.

A class for representing a shape.

### **Details**

This abstract class represents a shape, used for graphical representation.

Arguments to the constructor are:

label: A text label to associate with the shape.

color: A color, as a character string.

### Methods

#### **Public methods:**

- KeggShape\$new()
- KeggShape\$equals()
- KeggShape\$getLabel()
- KeggShape\$getColor()
- KeggShape\$getRgbColor()
- KeggShape\$draw()
- KeggShape\$clone()

Method new(): Initialize new instance.

```
/sage:
eggShane$new(lahel = NA ch
```

```
KeggShape$new(label = NA_character_, color = NA_character_)
Arguments:
```

```
label The text label to display.
 color The color to use.
 Returns: Nothing.
Method equals(): Test if this shape is the same as another.
 Usage:
 KeggShape$equals(other)
 Arguments:
 other The other shape to compare with.
 Returns: TRUE or FALSE.
Method getLabel(): Gets the label associated with this shape.
 Usage:
 KeggShape$getLabel()
 Returns: The label.
Method getColor(): Gets the color associated with this shape.
 Usage:
 KeggShape$getColor()
 Returns: The color name as a string.
Method getRgbColor(): Gets the RGB color associated with this shape.
 KeggShape$getRgbColor(alpha = 255)
 Arguments:
 alpha The value to use for the alpha channel when building the RGB color object.
 Returns: The color as an RGB color object.
Method draw(): Draw the shape on the current image.
 Usage:
 KeggShape$draw()
 Returns: None.
Method clone(): The objects of this class are cloneable with this method.
 KeggShape$clone(deep = FALSE)
 Arguments:
 deep Whether to make a deep clone.
```

#### See Also

KeggRect, KeggCircle.

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```
# Create a circle instance
c <- KeggCircle$new(x=12, y=5, r=3, label='MyCircle')

# Create a rectangle instance
r <- KeggRect$new(left=10, top=10, bottom=20, right=30, color='yellow')</pre>
```

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