Package ‘biodbLipidmaps’

May 20, 2024

Title  biodbLipidmaps, a library for connecting to the Lipidmaps Structure database

Version  1.10.0

Description  The biodbLipidmaps library provides access to the Lipidmaps Structure Database, using biodb package framework. It allows to retrieve entries by their accession number, and run web the services lmsdSearch and lmsdRecord.

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

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

biocViews  Software, Infrastructure, DataImport

License  AGPL-3

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

RoxygenNote  7.2.2

Collate  'LipidmapsStructureConn.R' 'LipidmapsStructureEntry.R'
         'package.R' 'zzz.R'

PackageStatus  Deprecated

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Description

The biodbLipidmaps library provides access to the Lipidmaps Structure Database, using biodb package framework. It allows to retrieve entries by their accession number, and run web the services lmsdSearch and lmsdRecord.

Details

See vignette intro: “ vignette('intro', package='biodbLipidmaps')”

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See Also

LipidmapsStructureConn.

LipidmapsStructureConn

Lipidmaps Structure connector class.

Details

Connector class for Lipidmaps Structure.

Super classes

biodb::BiodbConnBase -> biodb::BiodbConn -> LipidmapsStructureConn
Methods

Public methods:

• LipidmapsStructureConn$wsLmsdSearch()
• LipidmapsStructureConn$wsLmsd()
• LipidmapsStructureConn$wsLmsdRecord()
• LipidmapsStructureConn$clone()

Method wsLmsdSearch(): Calls LMSDSearch web service. See https://www.lipidmaps.org/data/structure/programmaticaccess.html for details.

Usage:
LipidmapsStructureConn$wsLmsdSearch(
    mode = NULL,
    output.mode = NULL,
    output.type = NULL,
    output.delimiter = NULL,
    output.quote = NULL,
    output.column.header = NULL,
    lmid = NULL,
    name = NULL,
    formula = NULL,
    search.type = NULL,
    smiles.string = NULL,
    exact.mass = NULL,
    exact.mass.offset = NULL,
    core.class = NULL,
    main.class = NULL,
    sub.class = NULL,
    retfmt = c("plain", "request", "parsed", "ids")
)

Arguments:

mode The search mode: 'ProcessStrSearch', 'ProcessTextSearch' or 'ProcessTextOntologySearch'. Compulsory.
optput.mode If set to 'File', will output a in format 'output.type', otherwise will output HTML.
output.type The output format: 'TSV', 'CSV' or 'SDF'.
output.delimiter The delimiter for TSV or CSV formats: 'Tab', 'Comma', 'Semicolon'.
output.quote If quotes are to be used: 'Yes' or 'No'.
output.column.header If header must be output: 'Yes' or 'No'.
lmid a Lipidmaps ID.
name The name to search for.
formula The chemical formula to search for.
search.type The search type: 'SubStructure' or 'ExactMatch'.
smiles.string A SMILES to search for.
exact.mass The mass to search for.
exact.mass.offset The tolerance on the mass search.
core.class  An integer number from 1 to 8.
main.class  An integer number. See Lipidmaps documentation.
sub.class  An integer number. See Lipidmaps documentation.

**retfmt** Use to set the format of the returned value. 'plain' will return the raw results from the server, as a character value. 'request' will return the request that would have been sent, as a BiodbRequest object. 'parsed' will return data frame. 'ids' will return a character vector containing the IDs of the matching entries.

**Returns:** Depending on 'retfmt'.

**Method** wsLmsd(): Calls LMSD web service for downloading one entry.

**Usage:**

```r
LipidmapsStructureConn$wsLmsd(
  lmid,
  format = c("tsv", "csv"),
  retfmt = c("plain", "request", "parsed")
)
```

**Arguments:**

- **lmid** The accession number of the entry to retrieve.
- **format** The output format (either 'tsv' or 'csv').
- **retfmt** Use to set the format of the returned value. 'plain' will return the raw results from the server, as a character value. 'request' will return the request that would have been sent, as a BiodbRequest object. 'parsed' will return data frame.

**Returns:** Depending on 'retfmt'.

**Method** wsLmsdRecord(): Calls LMSDRecord web service. See http://www.lipidmaps.org/data/structure/programmaticaccess.html.

**Usage:**

```r
LipidmapsStructureConn$wsLmsdRecord(
  lmid,
  mode = NULL,
  output.type = NULL,
  output.delimiter = NULL,
  output.quote = NULL,
  output.column.header = NULL,
  retfmt = c("plain", "request", "parsed")
)
```

**Arguments:**

- **lmid** A character vector containing the IDs of the wanted entries.
- **mode** If set to 'File', will output a in format 'output.type', otherwise will output HTML.
- **output.type** The output format: 'TSV', 'CSV' or 'SDF'.
- **output.delimiter** The delimiter for TSV or CSV formats: 'Tab', 'Comma', 'Semicolon'.
- **output.quote** If quotes are to be used: 'Yes' or 'No'.
- **output.column.header** If header must be output: 'Yes' or 'No'.
- **retfmt** Use to set the format of the returned value. 'plain' will return the raw results from the server, as a character value. 'request' will return the request that would have been sent, as a BiodbRequest object. 'parsed' will return data frame.
Returns: Depending on ‘retfmt’.

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

Usage:
LipidmapsStructureConn$clone(deep = FALSE)

Arguments:
deepl Whether to make a deep clone.

Examples

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

# Create a connector
conn <- mybiodb$getFactory()$createConn('lipidmaps.structure')

# Get an entry
e <- conn$getEntry('LMFA00000001')

# Terminate instance.
mybiodb$terminate()

LipidmapsStructureEntry

Lipidmaps Structure entry class.

Description

Lipidmaps Structure entry class.
Lipidmaps Structure entry class.

Details

Entry class for Lipidmaps Structure.

Super classes

biodb::BiodbEntry -> biodb::BiodbCsvEntry -> LipidmapsStructureEntry

Methods

Public methods:
• LipidmapsStructureEntry$new()
• LipidmapsStructureEntry$clone()

Method new(): New instance initializer. Entry classes must not be instantiated directly. Instead, you must use the getEntry() method of the connector class.
Usage:
LipidmapsStructureEntry$new(...)

Arguments:
... All parameters are passed to super class' initializer.

Returns: Nothing.

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

Usage:
LipidmapsStructureEntry$clone(deep = FALSE)

Arguments:
- deep: Whether to make a deep clone.

Examples

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

# Create a connector
conn <- mybiodb$getFactory()$createConn('lipidmaps.structure')

# Get an entry
e <- conn$getEntry('LMFA00000001')

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