# Package 'dbparser'

August 26, 2020

```
Description
      This tool is for parsing the 'DrugBank' XML database <a href="https://www.drugbank.ca/">https://www.drugbank.ca/</a>. The parsed
      data are then returned in a proper 'R' dataframe with the ability to save
      them in a given database.
License MIT + file LICENSE
Encoding UTF-8
LazyData true
Imports DBI, dplyr, odbc, progress, purrr, readr, RMariaDB, RSQLite,
      tibble, tools, XML
RoxygenNote 7.1.0
Suggests knitr, rmarkdown, testthat
VignetteBuilder knitr
URL https://docs.ropensci.org/dbparser/,
      https://github.com/ropensci/dbparser/
BugReports https://github.com/ropensci/dbparser/issues
Depends R (>= 2.10)
NeedsCompilation no
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Title 'DrugBank' Database XML Parser

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articles

Drugs/ Carriers/ Enzymes/ Targets/ Transporters articles element parser

# **Description**

Return a list of articles that were used as references for drugs carriers

```
drugs_articles(
  save_table = FALSE,
  save_csv = FALSE,
  csv_path = ".",
  override_csv = FALSE,
  database_connection = NULL
)
carriers_articles(
  save_table = FALSE,
  save_csv = FALSE,
  csv_path = ".",
 override_csv = FALSE,
  database\_connection = NULL
)
enzymes_articles(
  save_table = FALSE,
  save_csv = FALSE,
  csv_path = ".",
  override_csv = FALSE,
  database\_connection = NULL
)
targets_articles(
  save_table = FALSE,
```

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```
save_csv = FALSE,
  csv_path = ".",
  override_csv = FALSE,
  database_connection = NULL
)

transporters_articles(
  save_table = FALSE,
  save_csv = FALSE,
  csv_path = ".",
  override_csv = FALSE,
  database_connection = NULL
)
```

## Arguments

save\_table boolean, save table in database if true.

save\_csv boolean, save csv version of parsed tibble if true

csv\_path location to save csv files into it, default is current location, save\_csv must be

true

override\_csv override existing csv, if any, in case it is true in the new parse operation

database\_connection

DBI connection object that holds a connection to user defined database. If save\_table is enabled without providing value for this function an error will

be thrown.

#### Value

a tibble with 4 variables:

**ref-id** Identifier for the article being referenced. This is unique across all reference types (books, links, article, attachments).

**pubmed-id** The PubMed identifier for the article.

citation Article citation in a standard format.

parent\_id drug/carrier/target/enzyme/transporter id

## read\_drugbank\_xml\_db

read\_drugbank\_xml\_db function must be called first before any parser.

If read\_drugbank\_xml\_db is called before for any reason, so no need to call it again before calling this function.

#### See Also

Other references: attachments, books, links, references()

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# **Examples**

```
## Not run:
# the same parameters and usage will be applied for any parser
# return only the parsed tibble
run_all_parsers()
# will throw an error, as database_connection is NULL
run_all_parsers(save_table = TRUE)
# save in database in SQLite in memory database and return parsed tibble
sqlite_con <- DBI::dbConnect(RSQLite::SQLite())</pre>
run_all_parsers(save_table = TRUE, database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in current location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE)
# save in database, save parsed tibble as csv,
# if it does not exist in current location and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_table = TRUE, save_csv = TRUE,
database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in given location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE, csv_path = TRUE)
# save parsed tibble as csv if it does not exist in current location and
# return parsed tibble.
# if the csv exist override it and return it.
run_all_parsers(save_csv = TRUE, csv_path = TRUE, override = TRUE)
## End(Not run)
```

attachments

Drugs/ Carriers/ Enzymes/ Targets/ Transporters attachments element parser

## **Description**

Return a list of attachment that were used as references for drugs carriers

```
drugs_attachments(
  save_table = FALSE,
  save_csv = FALSE,
```

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```
csv_path = ".",
  override_csv = FALSE,
  database_connection = NULL
)
carriers_attachments(
  save_table = FALSE,
  save_csv = FALSE,
  csv_path = ".",
  override_csv = FALSE,
  database\_connection = NULL
)
enzymes_attachments(
  save_table = FALSE,
  save\_csv = FALSE,
  csv_path = ".",
  override_csv = FALSE,
  database_connection = NULL
targets_attachments(
  save_table = FALSE,
  save_csv = FALSE,
  csv_path = ".",
  override_csv = FALSE,
  database\_connection = NULL
)
transporters_attachments(
  save_table = FALSE,
  save_csv = FALSE,
  csv_path = ".",
  override_csv = FALSE,
  database\_connection = NULL
)
```

# **Arguments**

save\_table boolean, save table in database if true.

save\_csv boolean, save csv version of parsed tibble if true

csv\_path location to save csv files into it, default is current location, save\_csv must be

true

override\_csv override existing csv, if any, in case it is true in the new parse operation database\_connection

DBI connection object that holds a connection to user defined database. If save\_table is enabled without providing value for this function an error will be thrown.

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#### Value

```
a tibble with 4 variables:
```

**ref-id** Identifier for the article being referenced. This is unique across all reference types (books, links, article, attachments).

title The title of the attachment.

url The url to download the attachment from.

parent\_id drug/carrier/target/enzyme/transporter id

#### read\_drugbank\_xml\_db

read\_drugbank\_xml\_db function must be called first before any parser.

If read\_drugbank\_xml\_db is called before for any reason, so no need to call it again before calling this function.

#### See Also

Other references: articles, books, links, references()

```
## Not run:
# the same parameters and usage will be applied for any parser
# return only the parsed tibble
run_all_parsers()
# will throw an error, as database_connection is NULL
run_all_parsers(save_table = TRUE)
# save in database in SQLite in memory database and return parsed tibble
sqlite_con <- DBI::dbConnect(RSQLite::SQLite())</pre>
run_all_parsers(save_table = TRUE, database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in current location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE)
# save in database, save parsed tibble as csv,
# if it does not exist in current location and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_table = TRUE, save_csv = TRUE,
database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in given location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE, csv_path = TRUE)
# save parsed tibble as csv if it does not exist in current location and
```

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```
# return parsed tibble.
# if the csv exist override it and return it.
run_all_parsers(save_csv = TRUE, csv_path = TRUE, override = TRUE)
## End(Not run)
```

books

Drugs/ Carriers/ Enzymes/ Targets/ Transporters books element parser

# **Description**

Return a list of text books that were used as references for drugs, carriers, enzymes, targets or transporters

```
drugs_textbooks(
  save_table = FALSE,
  save_csv = FALSE,
  csv_path = ".",
  override_csv = FALSE,
  database\_connection = NULL
)
carriers_textbooks(
  save_table = FALSE,
  save_csv = FALSE,
  csv_path = ".",
 override_csv = FALSE,
  database_connection = NULL
)
enzymes_textbooks(
  save_table = FALSE,
  save\_csv = FALSE,
  csv_path = ".",
  override_csv = FALSE,
  database\_connection = NULL
)
targets_textbooks(
  save_table = FALSE,
  save\_csv = FALSE,
  csv_path = ".",
  override_csv = FALSE,
  database\_connection = NULL
```

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```
transporters_textbooks(
  save_table = FALSE,
  save_csv = FALSE,
  csv_path = ".",
  override_csv = FALSE,
  database_connection = NULL
)
```

## **Arguments**

save\_table boolean, save table in database if true.

save\_csv boolean, save csv version of parsed tibble if true

csv\_path location to save csv files into it, default is current location, save\_csv must be

true

override\_csv override existing csv, if any, in case it is true in the new parse operation

database\_connection

DBI connection object that holds a connection to user defined database. If save\_table is enabled without providing value for this function an error will be thrown.

# Value

a tibble with 4 variables:

**ref-id** Identifier for the article being referenced. This is unique across all reference types (books, links, article, attachments).

isbn ISBN identifying the textbook.

citation A Textbook citation in a standard format.

parent\_id drug/ carrier/ target/ enzyme/ transporter id

## read\_drugbank\_xml\_db

read\_drugbank\_xml\_db function must be called first before any parser.

If read\_drugbank\_xml\_db is called before for any reason, so no need to call it again before calling this function.

## See Also

```
Other references: articles, attachments, links, references()
```

```
## Not run:
# the same parameters and usage will be applied for any parser
# return only the parsed tibble
run_all_parsers()
```

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```
# will throw an error, as database_connection is NULL
run_all_parsers(save_table = TRUE)
# save in database in SQLite in memory database and return parsed tibble
sqlite_con <- DBI::dbConnect(RSQLite::SQLite())</pre>
run_all_parsers(save_table = TRUE, database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in current location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE)
# save in database, save parsed tibble as csv,
# if it does not exist in current location and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_table = TRUE, save_csv = TRUE,
database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in given location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE, csv_path = TRUE)
# save parsed tibble as csv if it does not exist in current location and
# return parsed tibble.
# if the csv exist override it and return it.
run_all_parsers(save_csv = TRUE, csv_path = TRUE, override = TRUE)
## End(Not run)
```

cett

Run all CETT related parsers

# Description

Run all parsers that retrieve carriers, enzymes, targets and transporters related information

```
cett(
  save_table = FALSE,
  save_csv = FALSE,
  csv_path = ".",
  override_csv = FALSE,
  database_connection = NULL
)
```

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# Arguments

save\_table boolean, save table in database if true.

save\_csv boolean, save csv version of parsed tibble if true

csv\_path location to save csv files into it, default is current location, save\_csv must be true

override\_csv override existing csv, if any, in case it is true in the new parse operation database\_connection

DBI connection object that holds a connection to user defined database. If save\_table is enabled without providing value for this function an error will be thrown.

#### Value

a list of all drugs parsed tibbles

# read\_drugbank\_xml\_db

read\_drugbank\_xml\_db function must be called first before any parser.

If read\_drugbank\_xml\_db is called before for any reason, so no need to call it again before calling this function.

#### See Also

```
Other collective_parsers: drugs(), run_all_parsers()
```

```
## Not run:
# the same parameters and usage will be applied for any parser
# return only the parsed tibble
run_all_parsers()
# will throw an error, as database_connection is NULL
run_all_parsers(save_table = TRUE)
# save in database in SQLite in memory database and return parsed tibble
sqlite_con <- DBI::dbConnect(RSQLite::SQLite())</pre>
run_all_parsers(save_table = TRUE, database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in current location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE)
# save in database, save parsed tibble as csv,
# if it does not exist in current location and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_table = TRUE, save_csv = TRUE,
database_connection = sqlite_con)
```

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```
# save parsed tibble as csv if it does not exist in given location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE, csv_path = TRUE)

# save parsed tibble as csv if it does not exist in current location and
# return parsed tibble.
# if the csv exist override it and return it.
run_all_parsers(save_csv = TRUE, csv_path = TRUE, override = TRUE)

## End(Not run)
```

cett\_actions\_doc

Carriers/ Enzymes/ Targets/ Transporters Actions parsers

## **Description**

Collection of related actions

```
carriers_actions(
  save_table = FALSE,
  save_csv = FALSE,
  csv_path = ".",
  override_csv = FALSE,
  database_connection = NULL
)
enzymes_actions(
  save_table = FALSE,
  save_csv = FALSE,
  csv_path = ".",
  override_csv = FALSE,
  database_connection = NULL
)
targets_actions(
  save_table = FALSE,
  save_csv = FALSE,
  csv_path = ".",
  override_csv = FALSE,
  database_connection = NULL
)
transporters_actions(
  save_table = FALSE,
```

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```
save_csv = FALSE,
  csv_path = ".",
  override_csv = FALSE,
  database_connection = NULL
)
```

## **Arguments**

save\_table boolean, save table in database if true.

save\_csv boolean, save csv version of parsed tibble if true

csv\_path location to save csv files into it, default is current location, save\_csv must be

true

override\_csv override existing csv, if any, in case it is true in the new parse operation

database\_connection

DBI connection object that holds a connection to user defined database. If save\_table is enabled without providing value for this function an error will

be thrown.

#### Value

a tibble with 2 variables:

action describe related action

parent\_id carrier/ target/ enzyme/ transporter id

## read\_drugbank\_xml\_db

read\_drugbank\_xml\_db function must be called first before any parser.

If read\_drugbank\_xml\_db is called before for any reason, so no need to call it again before calling this function.

#### See Also

```
Other cett: cett_doc, cett_ex_identity_doc, cett_go_doc, cett_poly_doc, cett_poly_pfms_doc, cett_poly_syn_doc
```

```
## Not run:
# the same parameters and usage will be applied for any parser
# return only the parsed tibble
run_all_parsers()

# will throw an error, as database_connection is NULL
run_all_parsers(save_table = TRUE)

# save in database in SQLite in memory database and return parsed tibble
sqlite_con <- DBI::dbConnect(RSQLite::SQLite())
run_all_parsers(save_table = TRUE, database_connection = sqlite_con)</pre>
```

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```
# save parsed tibble as csv if it does not exist in current location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE)
# save in database, save parsed tibble as csv,
# if it does not exist in current location and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_table = TRUE, save_csv = TRUE,
database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in given location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE, csv_path = TRUE)
# save parsed tibble as csv if it does not exist in current location and
# return parsed tibble.
# if the csv exist override it and return it.
run_all_parsers(save_csv = TRUE, csv_path = TRUE, override = TRUE)
## End(Not run)
```

cett\_doc

Carriers/ Enzymes/ Targets/ Transporters parsers

# **Description**

Protein targets of drug action, enzymes that are inhibited/induced or involved in metabolism, and carrier or transporter proteins involved in movement of the drug across biological membranes.

```
carriers(
   save_table = FALSE,
   save_csv = FALSE,
   csv_path = ".",
   override_csv = FALSE,
   database_connection = NULL
)

enzymes(
   save_table = FALSE,
   save_csv = FALSE,
   csv_path = ".",
   override_csv = FALSE,
   database_connection = NULL
)
```

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```
targets(
  save_table = FALSE,
  save_csv = FALSE,
  csv_path = ".",
  override_csv = FALSE,
  database_connection = NULL
)

transporters(
  save_table = FALSE,
   save_csv = FALSE,
   csv_path = ".",
  override_csv = FALSE,
  database_connection = NULL
)
```

#### **Arguments**

save\_table boolean, save table in database if true.

save\_csv boolean, save csv version of parsed tibble if true

csv\_path location to save csv files into it, default is current location, save\_csv must be

true

override\_csv override existing csv, if any, in case it is true in the new parse operation

database\_connection

DBI connection object that holds a connection to user defined database. If save\_table is enabled without providing value for this function an error will be thrown.

# Value

a tibble with 6 variables (8 for enzymes):

id Universal Protein Resource (UniProt) Identifier for the record

name related name

organism Organism that the protein comes from.

known\_action Whether the pharmacological action of the drug is due to this target interaction.

**inhibition-strength** Whether the strength of enzyme inhibition is strong, moderate, or unknown. **Only applies to enzymes** 

induction-strength Whether the strength of enzyme induction is strong or unknown. Only applies to enzymes

position related position

parent\_id drugbank id

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#### read\_drugbank\_xml\_db

read\_drugbank\_xml\_db function must be called first before any parser.

If read\_drugbank\_xml\_db is called before for any reason, so no need to call it again before calling this function.

#### See Also

Other cett: cett\_actions\_doc, cett\_ex\_identity\_doc, cett\_go\_doc, cett\_poly\_doc, cett\_poly\_pfms\_doc, cett\_poly\_syn\_doc

```
## Not run:
# the same parameters and usage will be applied for any parser
# return only the parsed tibble
run_all_parsers()
# will throw an error, as database_connection is NULL
run_all_parsers(save_table = TRUE)
# save in database in SQLite in memory database and return parsed tibble
sqlite_con <- DBI::dbConnect(RSQLite::SQLite())</pre>
run_all_parsers(save_table = TRUE, database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in current location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE)
# save in database, save parsed tibble as csv,
# if it does not exist in current location and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_table = TRUE, save_csv = TRUE,
database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in given location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE, csv_path = TRUE)
# save parsed tibble as csv if it does not exist in current location and
# return parsed tibble.
# if the csv exist override it and return it.
run_all_parsers(save_csv = TRUE, csv_path = TRUE, override = TRUE)
## End(Not run)
```

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# **Description**

Extract descriptions of identified polypeptide external identifiers for targets, enzymes, carriers, or transporters.

# Usage

```
carriers_polypep_ex_ident(
  save_table = FALSE,
  save\_csv = FALSE,
  csv_path = ".",
  override_csv = FALSE,
  database_connection = NULL
)
enzymes_polypep_ex_ident(
  save_table = FALSE,
  save\_csv = FALSE,
  csv_path = ".",
  override_csv = FALSE,
  database_connection = NULL
)
targets_polypep_ex_ident(
  save_table = FALSE,
  save_csv = FALSE,
  csv_path = ".",
  override_csv = FALSE,
  database_connection = NULL
)
transporters_polypep_ex_ident(
  save_table = FALSE,
  save_csv = FALSE,
  csv_path = ".",
  override_csv = FALSE,
  database_connection = NULL
)
```

# Arguments

save\_table boolean, save table in database if true.
save\_csv boolean, save csv version of parsed tibble if true

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csv\_path location to save csv files into it, default is current location, save\_csv must be

true

override\_csv override existing csv, if any, in case it is true in the new parse operation database\_connection

DBI connection object that holds a connection to user defined database. If save\_table is enabled without providing value for this function an error will be thrown.

#### Value

a tibble with 3 variables:

resource Name of the source database.

identifier Identifier for this drug in the given resource.

parent\_key polypeptide id

# read\_drugbank\_xml\_db

read\_drugbank\_xml\_db function must be called first before any parser.

If read\_drugbank\_xml\_db is called before for any reason, so no need to call it again before calling this function.

#### See Also

```
Other cett: cett_actions_doc, cett_doc, cett_go_doc, cett_poly_doc, cett_poly_pfms_doc, cett_poly_syn_doc
```

```
## Not run:
# the same parameters and usage will be applied for any parser
# return only the parsed tibble
run_all_parsers()
# will throw an error, as database_connection is NULL
run_all_parsers(save_table = TRUE)
# save in database in SQLite in memory database and return parsed tibble
sqlite_con <- DBI::dbConnect(RSQLite::SQLite())</pre>
run_all_parsers(save_table = TRUE, database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in current location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE)
# save in database, save parsed tibble as csv,
# if it does not exist in current location and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_table = TRUE, save_csv = TRUE,
```

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```
database_connection = sqlite_con)

# save parsed tibble as csv if it does not exist in given location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE, csv_path = TRUE)

# save parsed tibble as csv if it does not exist in current location and
# return parsed tibble.
# if the csv exist override it and return it.
run_all_parsers(save_csv = TRUE, csv_path = TRUE, override = TRUE)

## End(Not run)
```

cett\_go\_doc

Carriers/ Enzymes/ Targets/ Transporters Polypeptide GO Classifier parsers

# **Description**

Extract descriptions of identified polypeptide go classifier for targets, enzymes, carriers, or transporters.

```
carriers_polypeptides_go(
  save_table = FALSE,
  save\_csv = FALSE,
  csv_path = ".",
  override_csv = FALSE,
  database_connection = NULL
)
enzymes_polypeptides_go(
  save_table = FALSE,
  save_csv = FALSE,
  csv_path = ".",
  override_csv = FALSE,
  database_connection = NULL
)
targets_polypeptides_go(
  save_table = FALSE,
  save_csv = FALSE,
  csv_path = ".",
  override_csv = FALSE,
  database_connection = NULL
)
```

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```
transporters_polypeptides_go(
  save_table = FALSE,
  save_csv = FALSE,
  csv_path = ".",
  override_csv = FALSE,
  database_connection = NULL
)
```

# Arguments

save\_table boolean, save table in database if true.

save\_csv boolean, save csv version of parsed tibble if true

csv\_path location to save csv files into it, default is current location, save\_csv must be

true

override\_csv override existing csv, if any, in case it is true in the new parse operation

database\_connection

DBI connection object that holds a connection to user defined database. If save\_table is enabled without providing value for this function an error will be thrown.

#### Value

```
a tibble with 3 variables:
```

category

description

parent\_key polypeptide id

# read\_drugbank\_xml\_db

read\_drugbank\_xml\_db function must be called first before any parser.

If read\_drugbank\_xml\_db is called before for any reason, so no need to call it again before calling this function.

#### See Also

```
Other cett: cett_actions_doc, cett_doc, cett_ex_identity_doc, cett_poly_doc, cett_poly_pfms_doc, cett_poly_syn_doc
```

```
## Not run:
# the same parameters and usage will be applied for any parser
# return only the parsed tibble
run_all_parsers()
# will throw an error, as database_connection is NULL
```

cett\_poly\_doc 21

```
run_all_parsers(save_table = TRUE)
# save in database in SQLite in memory database and return parsed tibble
sqlite_con <- DBI::dbConnect(RSQLite::SQLite())</pre>
run_all_parsers(save_table = TRUE, database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in current location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE)
# save in database, save parsed tibble as csv,
# if it does not exist in current location and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_table = TRUE, save_csv = TRUE,
database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in given location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE, csv_path = TRUE)
# save parsed tibble as csv if it does not exist in current location and
# return parsed tibble.
# if the csv exist override it and return it.
run_all_parsers(save_csv = TRUE, csv_path = TRUE, override = TRUE)
## End(Not run)
```

cett\_poly\_doc

Carriers/ Enzymes/ Targets/ Transporters Polypeptide parsers

# **Description**

Extract descriptions of identified polypeptide targets, enzymes, carriers, or transporters.

```
carriers_polypeptides(
   save_table = FALSE,
   save_csv = FALSE,
   csv_path = ".",
   override_csv = FALSE,
   database_connection = NULL
)
enzymes_polypeptides(
   save_table = FALSE,
   save_csv = FALSE,
```

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```
csv_path = ".",
 override_csv = FALSE,
  database_connection = NULL
)
targets_polypeptides(
  save_table = FALSE,
  save_csv = FALSE,
 csv_path = ".",
 override_csv = FALSE,
  database_connection = NULL
)
transporters_polypeptides(
  save_table = FALSE,
  save\_csv = FALSE,
  csv_path = ".",
 override_csv = FALSE,
  database_connection = NULL
)
```

#### Arguments

save\_table boolean, save table in database if true.

save\_csv boolean, save csv version of parsed tibble if true

csv\_path location to save csv files into it, default is current location, save\_csv must be

true

override\_csv override existing csv, if any, in case it is true in the new parse operation

database\_connection

DBI connection object that holds a connection to user defined database. If save\_table is enabled without providing value for this function an error will be thrown.

# Value

a tibble with 20 variables:

## id Universal Protein Resource (UniProt) identifier

**source** Specifies whether the identified polypeptide ID is associated with any of the following UniProt knowledge bases: Swiss-Prot, which is manually annotated and reviewed, or TrEMBL, which is automatically annotated and not reviewed.

## name

general\_function General summary of the physiological function of the polypeptide

**specific\_function** A more specific description of the polypeptide's physiological function within the cell.

**gene\_name** The short name commonly associated with the associated gene. Eg. PTGS1.

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**locus** The specific chromosomal location or position of the gene's sequence on a chromosome.

cellular\_location The cellular location of the polypeptide.

**transmembrane\_regions** Areas of the polypeptide sequence that span a biological membrane.

signal\_regions Location of any signal peptides within the polypeptide sequence.

theoretical\_pi Theoretical isoelectric point.

molecular\_weight The molecular weight of the polypeptide.

**chromosome\_location** The chromosomal location of the polypeptide gene

**organism** The organism in which this polypeptide functions.

organism\_ncbi\_taxonomy\_id

amino\_acid\_sequence The amino acid sequence of the polypeptide

amino acid format

**gene\_sequence** The sequence of the associated gene.

gene format

parent\_key carrier/ target/ enzyme/ transporter id

# read\_drugbank\_xml\_db

read\_drugbank\_xml\_db function must be called first before any parser.

If read\_drugbank\_xml\_db is called before for any reason, so no need to call it again before calling this function.

#### See Also

```
Other cett: cett_actions_doc, cett_doc, cett_ex_identity_doc, cett_go_doc, cett_poly_pfms_doc, cett_poly_syn_doc
```

```
## Not run:
# the same parameters and usage will be applied for any parser
# return only the parsed tibble
run_all_parsers()

# will throw an error, as database_connection is NULL
run_all_parsers(save_table = TRUE)

# save in database in SQLite in memory database and return parsed tibble
sqlite_con <- DBI::dbConnect(RSQLite::SQLite())
run_all_parsers(save_table = TRUE, database_connection = sqlite_con)

# save parsed tibble as csv if it does not exist in current location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE)

# save in database, save parsed tibble as csv,</pre>
```

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```
# if it does not exist in current location and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_table = TRUE, save_csv = TRUE,
database_connection = sqlite_con)

# save parsed tibble as csv if it does not exist in given location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE, csv_path = TRUE)

# save parsed tibble as csv if it does not exist in current location and
# return parsed tibble.
# if the csv exist override it and return it.
run_all_parsers(save_csv = TRUE, csv_path = TRUE, override = TRUE)

## End(Not run)
```

cett\_poly\_pfms\_doc

Carriers/ Enzymes/ Targets/ Transporters Polypeptide PFAMS parsers

# **Description**

Extract descriptions of identified polypeptide PFAMS targets, enzymes, carriers, or transporters.

```
carriers_polypeptides_pfams(
  save_table = FALSE,
  save\_csv = FALSE,
  csv_path = ".",
  override_csv = FALSE,
  database connection = NULL
)
enzymes_polypeptides_pfams(
  save_table = FALSE,
  save_csv = FALSE,
  csv_path = ".",
  override_csv = FALSE,
  database_connection = NULL
)
targets_polypeptides_pfams(
  save_table = FALSE,
  save\_csv = FALSE,
  csv_path = ".",
  override_csv = FALSE,
  database\_connection = NULL
```

cett\_poly\_pfms\_doc 25

```
transporters_polypeptides_pfams(
   save_table = FALSE,
   save_csv = FALSE,
   csv_path = ".",
   override_csv = FALSE,
   database_connection = NULL
)
```

## **Arguments**

save\_table boolean, save table in database if true.

save\_csv boolean, save csv version of parsed tibble if true

csv\_path location to save csv files into it, default is current location, save\_csv must be

true

override\_csv override existing csv, if any, in case it is true in the new parse operation

database\_connection

DBI connection object that holds a connection to user defined database. If save\_table is enabled without providing value for this function an error will be thrown.

## Value

a tibble with 3 variables:

name The sequence of the associated gene.

identifier

parent\_key polypeptide id

# read\_drugbank\_xml\_db

read\_drugbank\_xml\_db function must be called first before any parser.

If read\_drugbank\_xml\_db is called before for any reason, so no need to call it again before calling this function.

#### See Also

```
Other\ cett:\ cett\_actions\_doc,\ cett\_doc,\ cett\_ex\_identity\_doc,\ cett\_go\_doc,\ cett\_poly\_doc,\ cett\_poly\_syn\_doc
```

```
## Not run:
# the same parameters and usage will be applied for any parser
# return only the parsed tibble
run_all_parsers()
```

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```
# will throw an error, as database_connection is NULL
run_all_parsers(save_table = TRUE)
# save in database in SQLite in memory database and return parsed tibble
sqlite_con <- DBI::dbConnect(RSQLite::SQLite())</pre>
run_all_parsers(save_table = TRUE, database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in current location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE)
# save in database, save parsed tibble as csv,
# if it does not exist in current location and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_table = TRUE, save_csv = TRUE,
database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in given location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE, csv_path = TRUE)
# save parsed tibble as csv if it does not exist in current location and
# return parsed tibble.
# if the csv exist override it and return it.
run_all_parsers(save_csv = TRUE, csv_path = TRUE, override = TRUE)
## End(Not run)
```

cett\_poly\_syn\_doc

Carriers/ Enzymes/ Targets/ Transporters Polypeptide Synonyms parsers

# **Description**

Extract descriptions of identified polypeptide synonyms for targets, enzymes, carriers, or transporters.

```
carriers_polypeptides_syn(
  save_table = FALSE,
  save_csv = FALSE,
  csv_path = ".",
  override_csv = FALSE,
  database_connection = NULL
)
```

cett\_poly\_syn\_doc 27

```
enzymes_polypeptides_syn(
  save_table = FALSE,
  save\_csv = FALSE,
 csv_path = ".",
 override_csv = FALSE,
 database\_connection = NULL
)
targets_polypeptides_syn(
  save_table = FALSE,
  save_csv = FALSE,
 csv_path = ".",
 override_csv = FALSE,
 database_connection = NULL
)
transporters_polypeptides_syn(
  save_table = FALSE,
  save_csv = FALSE,
  csv_path = ".",
 override_csv = FALSE,
 database_connection = NULL
)
```

# Arguments

save\_table boolean, save table in database if true.

save\_csv boolean, save csv version of parsed tibble if true

csv\_path location to save csv files into it, default is current location, save\_csv must be

true

override\_csv override existing csv, if any, in case it is true in the new parse operation

database\_connection

DBI connection object that holds a connection to user defined database. If save\_table is enabled without providing value for this function an error will be thrown.

## Value

```
a tibble with 2 variables:
```

synonym

parent\_key polypeptide id

# read\_drugbank\_xml\_db

read\_drugbank\_xml\_db function must be called first before any parser.

If read\_drugbank\_xml\_db is called before for any reason, so no need to call it again before calling this function.

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# See Also

Other cett: cett\_actions\_doc, cett\_doc, cett\_ex\_identity\_doc, cett\_go\_doc, cett\_poly\_doc, cett\_poly\_pfms\_doc

## **Examples**

```
## Not run:
# the same parameters and usage will be applied for any parser
# return only the parsed tibble
run_all_parsers()
# will throw an error, as database_connection is NULL
run_all_parsers(save_table = TRUE)
# save in database in SQLite in memory database and return parsed tibble
sqlite_con <- DBI::dbConnect(RSQLite::SQLite())</pre>
run_all_parsers(save_table = TRUE, database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in current location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE)
# save in database, save parsed tibble as csv,
# if it does not exist in current location and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_table = TRUE, save_csv = TRUE,
database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in given location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE, csv_path = TRUE)
# save parsed tibble as csv if it does not exist in current location and
# return parsed tibble.
# if the csv exist override it and return it.
run_all_parsers(save_csv = TRUE, csv_path = TRUE, override = TRUE)
## End(Not run)
```

dbparser

dbparser: A package for reading and parsing **DrugBank** xml database.

#### **Description**

The main purpose of the 'dbparser' package is to parse [DrugBank](https://www.drugbank.ca/) database which is downloadable in XML format from [this link](https://www.DrugBank.ca/releases/latest).

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## **Details**

The parsed data can then be explored and analyzed as desired by the user with the ability to save parsed data into desired database as well.

To achieve this purpose, 'dbparser" package provides three main categories of functions:

- xml db reader,
- DrugBank elements parsers,
- and database related methods.

For more information kindly check the reference/index (https://docs.ropensci.org/dbparser/reference/index.html)

#### xml db reader functions

Reads DrugBank xml database and build drug elements full tree in memory

## parsers functions

Each parser function is responsible of parsing certain drug element and returning its tibble with the ability to save it in a predefined database.

Check this tutorial (https://docs.ropensci.org/dbparser/articles/dbparser.html)

#### database functions

To open a connection to given database in order to store parsed DrugBank elements database.

Check this tutorial (https://docs.ropensci.org/dbparser/articles/Database\_Saving.html)

drugs

Run all drug related parsers

# Description

Run all parsers that retrieve drugs related information

```
drugs(
   save_table = FALSE,
   save_csv = FALSE,
   csv_path = ".",
   override_csv = FALSE,
   database_connection = NULL
)
```

30 drugs

## Arguments

save\_table boolean, save table in database if true.

save\_csv boolean, save csv version of parsed tibble if true

save\_nath boolean to save say files into it, default is current leastic

csv\_path location to save csv files into it, default is current location, save\_csv must be

true

override\_csv override existing csv, if any, in case it is true in the new parse operation

database\_connection

DBI connection object that holds a connection to user defined database. If save\_table is enabled without providing value for this function an error will be thrown.

#### Value

a list of all drugs parsed tibbles

# read\_drugbank\_xml\_db

read\_drugbank\_xml\_db function must be called first before any parser.

If read\_drugbank\_xml\_db is called before for any reason, so no need to call it again before calling this function.

#### See Also

```
Other collective_parsers: cett(), run_all_parsers()
```

```
## Not run:
# the same parameters and usage will be applied for any parser
# return only the parsed tibble
run_all_parsers()
# will throw an error, as database_connection is NULL
run_all_parsers(save_table = TRUE)
# save in database in SQLite in memory database and return parsed tibble
sqlite_con <- DBI::dbConnect(RSQLite::SQLite())</pre>
run_all_parsers(save_table = TRUE, database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in current location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE)
# save in database, save parsed tibble as csv,
# if it does not exist in current location and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_table = TRUE, save_csv = TRUE,
database_connection = sqlite_con)
```

```
# save parsed tibble as csv if it does not exist in given location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE, csv_path = TRUE)
# save parsed tibble as csv if it does not exist in current location and
# return parsed tibble.
# if the csv exist override it and return it.
run_all_parsers(save_csv = TRUE, csv_path = TRUE, override = TRUE)
## End(Not run)
```

drug\_affected\_organisms

Drug Affected Organism parser

## **Description**

Organisms in which the drug may display activity; activity may depend on local susceptibility patterns and resistance.

#### Usage

```
drug_affected_organisms(
  save_table = FALSE,
  save_csv = FALSE,
  csv_path = ".",
  override_csv = FALSE,
  database_connection = NULL
)
```

# **Arguments**

save\_table boolean, save table in database if true.

save\_csv boolean, save csv version of parsed tibble if true

csv\_path location to save csv files into it, default is current location, save\_csv must be

true

override\_csv override existing csv, if any, in case it is true in the new parse operation

database\_connection

DBI connection object that holds a connection to user defined database. If save\_table is enabled without providing value for this function an error will be thrown.

#### Value

```
a tibble with 2 variables:

affected-organism affected-organism name

drugbank_id drugbank id
```

#### read\_drugbank\_xml\_db

```
read_drugbank_xml_db function must be called first before any parser.
```

If read\_drugbank\_xml\_db is called before for any reason, so no need to call it again before calling this function.

#### See Also

```
Other drugs: drug_ahfs_codes(), drug_atc_codes(), drug_calc_prop(), drug_categories(), drug_classification(), drug_dosages(), drug_ex_identity(), drug_exp_prop(), drug_external_links(), drug_food_interactions(), drug_general_information(), drug_groups(), drug_interactions(), drug_intern_brand(), drug_manufacturers(), drug_mixtures(), drug_packagers(), drug_patents(), drug_pdb_entries(), drug_pharmacology(), drug_prices(), drug_products(), drug_reactions_enzymes(), drug_reactions(), drug_salts(), drug_sequences(), drug_snp_adverse_reactions(), drug_snp_effects(), drug_syn()
```

```
## Not run:
# the same parameters and usage will be applied for any parser
# return only the parsed tibble
run_all_parsers()
# will throw an error, as database_connection is NULL
run_all_parsers(save_table = TRUE)
# save in database in SQLite in memory database and return parsed tibble
sqlite_con <- DBI::dbConnect(RSQLite::SQLite())</pre>
run_all_parsers(save_table = TRUE, database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in current location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE)
# save in database, save parsed tibble as csv,
# if it does not exist in current location and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_table = TRUE, save_csv = TRUE,
database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in given location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE, csv_path = TRUE)
```

drug\_ahfs\_codes 33

```
# save parsed tibble as csv if it does not exist in current location and
# return parsed tibble.
# if the csv exist override it and return it.
run_all_parsers(save_csv = TRUE, csv_path = TRUE, override = TRUE)
## End(Not run)
```

drug\_ahfs\_codes

Drug ahfs-codes parser

## **Description**

The American Hospital Formulary Service (AHFS) identifier for this drug.

## Usage

```
drug_ahfs_codes(
   save_table = FALSE,
   save_csv = FALSE,
   csv_path = ".",
   override_csv = FALSE,
   database_connection = NULL
)
```

# **Arguments**

save\_table boolean, save table in database if true.

save\_csv boolean, save csv version of parsed tibble if true

csv\_path location to save csv files into it, default is current location, save\_csv must be

true

override\_csv override existing csv, if any, in case it is true in the new parse operation

database\_connection

DBI connection object that holds a connection to user defined database. If save\_table is enabled without providing value for this function an error will be thrown.

## Value

a tibble with the following variables:

#### ahfs-code

drugbank\_id drugbank id

34 drug\_ahfs\_codes

#### read\_drugbank\_xml\_db

read\_drugbank\_xml\_db function must be called first before any parser.

If read\_drugbank\_xml\_db is called before for any reason, so no need to call it again before calling this function.

#### See Also

```
Other drugs: drug_affected_organisms(), drug_atc_codes(), drug_calc_prop(), drug_categories(), drug_classification(), drug_dosages(), drug_ex_identity(), drug_exp_prop(), drug_external_links(), drug_food_interactions(), drug_general_information(), drug_groups(), drug_interactions(), drug_intern_brand(), drug_manufacturers(), drug_mixtures(), drug_packagers(), drug_patents(), drug_pdb_entries(), drug_pharmacology(), drug_prices(), drug_products(), drug_reactions_enzymes(), drug_reactions(), drug_salts(), drug_sequences(), drug_snp_adverse_reactions(), drug_snp_effects(), drug_syn()
```

```
## Not run:
# the same parameters and usage will be applied for any parser
# return only the parsed tibble
run_all_parsers()
# will throw an error, as database_connection is NULL
run_all_parsers(save_table = TRUE)
# save in database in SQLite in memory database and return parsed tibble
sqlite_con <- DBI::dbConnect(RSQLite::SQLite())</pre>
run_all_parsers(save_table = TRUE, database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in current location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE)
# save in database, save parsed tibble as csv,
# if it does not exist in current location and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_table = TRUE, save_csv = TRUE,
database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in given location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE, csv_path = TRUE)
# save parsed tibble as csv if it does not exist in current location and
# return parsed tibble.
# if the csv exist override it and return it.
run_all_parsers(save_csv = TRUE, csv_path = TRUE, override = TRUE)
## End(Not run)
```

drug\_atc\_codes 35

drug\_atc\_codes

Drug ATC Codes element parser

## **Description**

The Anatomical Therapeutic Classification (ATC) code for the drug assigned by the World Health Organization Anatomical Chemical Classification System.

## Usage

```
drug_atc_codes(
   save_table = FALSE,
   save_csv = FALSE,
   csv_path = ".",
   override_csv = FALSE,
   database_connection = NULL
)
```

# Arguments

save\_table boolean, save table in database if true.

save\_csv boolean, save csv version of parsed tibble if true

csv\_path location to save csv files into it, default is current location, save\_csv must be

true

override\_csv override existing csv, if any, in case it is true in the new parse operation

database\_connection

DBI connection object that holds a connection to user defined database. If save\_table is enabled without providing value for this function an error will be thrown.

#### **Details**

Each 'atc-code" row has one or more level. The atc-code and level> have a code the code assigned by the World Health Organization Anatomical Therapeutic Chemical Classification system.

#### Value

a tibble with 10 variables

## read\_drugbank\_xml\_db

read\_drugbank\_xml\_db function must be called first before any parser.

If read\_drugbank\_xml\_db is called before for any reason, so no need to call it again before calling this function.

36 drug\_calc\_prop

#### See Also

```
Other drugs: drug_affected_organisms(), drug_ahfs_codes(), drug_calc_prop(), drug_categories(), drug_classification(), drug_dosages(), drug_ex_identity(), drug_exp_prop(), drug_external_links(), drug_food_interactions(), drug_general_information(), drug_groups(), drug_interactions(), drug_intern_brand(), drug_manufacturers(), drug_mixtures(), drug_packagers(), drug_patents(), drug_pdb_entries(), drug_pharmacology(), drug_prices(), drug_products(), drug_reactions_enzymes(), drug_reactions(), drug_salts(), drug_sequences(), drug_snp_adverse_reactions(), drug_snp_effects(), drug_syn()
```

```
## Not run:
# the same parameters and usage will be applied for any parser
# return only the parsed tibble
run_all_parsers()
# will throw an error, as database_connection is NULL
run_all_parsers(save_table = TRUE)
# save in database in SQLite in memory database and return parsed tibble
sqlite_con <- DBI::dbConnect(RSQLite::SQLite())</pre>
run_all_parsers(save_table = TRUE, database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in current location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE)
# save in database, save parsed tibble as csv,
# if it does not exist in current location and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_table = TRUE, save_csv = TRUE,
database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in given location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE, csv_path = TRUE)
# save parsed tibble as csv if it does not exist in current location and
# return parsed tibble.
# if the csv exist override it and return it.
run_all_parsers(save_csv = TRUE, csv_path = TRUE, override = TRUE)
## End(Not run)
```

drug\_calc\_prop 37

# **Description**

Drug properties that have been predicted by ChemAxon or ALOGPS based on the inputed chemical structure. Associated links below will redirect to descriptions of the specific term.

## Usage

```
drug_calc_prop(
  save_table = FALSE,
  save_csv = FALSE,
  csv_path = ".",
  override_csv = FALSE,
  database_connection = NULL
)
```

## **Arguments**

save\_table boolean, save table in database if true.

save\_csv boolean, save csv version of parsed tibble if true

csv\_path location to save csv files into it, default is current location, save\_csv must be

true

override\_csv override existing csv, if any, in case it is true in the new parse operation

database\_connection

DBI connection object that holds a connection to user defined database. If save\_table is enabled without providing value for this function an error will be thrown.

# Value

a tibble with 4 variables:

kind Name of the property.

**value** Predicted physicochemical properties; obtained by the use of prediction software such as ALGOPS and ChemAxon.

source Name of the software used to calculate this property, either ChemAxon or ALOGPS.

drugbank\_id drugbank id

## read\_drugbank\_xml\_db

read\_drugbank\_xml\_db function must be called first before any parser.

If read\_drugbank\_xml\_db is called before for any reason, so no need to call it again before calling this function.

38 drug\_categories

### See Also

```
Other drugs: drug_affected_organisms(), drug_ahfs_codes(), drug_atc_codes(), drug_categories(), drug_classification(), drug_dosages(), drug_ex_identity(), drug_exp_prop(), drug_external_links(), drug_food_interactions(), drug_general_information(), drug_groups(), drug_interactions(), drug_intern_brand(), drug_manufacturers(), drug_mixtures(), drug_packagers(), drug_patents(), drug_pdb_entries(), drug_pharmacology(), drug_prices(), drug_products(), drug_reactions_enzymes(), drug_reactions(), drug_salts(), drug_sequences(), drug_snp_adverse_reactions(), drug_snp_effects(), drug_syn()
```

```
## Not run:
# the same parameters and usage will be applied for any parser
# return only the parsed tibble
run_all_parsers()
# will throw an error, as database_connection is NULL
run_all_parsers(save_table = TRUE)
# save in database in SQLite in memory database and return parsed tibble
sqlite_con <- DBI::dbConnect(RSQLite::SQLite())</pre>
run_all_parsers(save_table = TRUE, database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in current location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE)
# save in database, save parsed tibble as csv,
# if it does not exist in current location and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_table = TRUE, save_csv = TRUE,
database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in given location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE, csv_path = TRUE)
# save parsed tibble as csv if it does not exist in current location and
# return parsed tibble.
# if the csv exist override it and return it.
run_all_parsers(save_csv = TRUE, csv_path = TRUE, override = TRUE)
## End(Not run)
```

drug\_categories 39

# **Description**

General categorizations of the drug.

### **Usage**

```
drug_categories(
  save_table = FALSE,
  save_csv = FALSE,
  csv_path = ".",
  override_csv = FALSE,
  database_connection = NULL
)
```

#### **Arguments**

save\_table boolean, save table in database if true.

save\_csv boolean, save csv version of parsed tibble if true

csv\_path location to save csv files into it, default is current location, save\_csv must be

true

override\_csv override existing csv, if any, in case it is true in the new parse operation

database\_connection

DBI connection object that holds a connection to user defined database. If save\_table is enabled without providing value for this function an error will

be thrown.

### Value

```
a tibble with 2 variables:
```

```
category category name
```

mesh-id The Medical Subjects Headings (MeSH) identifier for the category.

drugbank\_id drugbank id

# read\_drugbank\_xml\_db

read\_drugbank\_xml\_db function must be called first before any parser.

If read\_drugbank\_xml\_db is called before for any reason, so no need to call it again before calling this function.

## See Also

```
Other drugs: drug_affected_organisms(), drug_ahfs_codes(), drug_atc_codes(), drug_calc_prop(), drug_classification(), drug_dosages(), drug_ex_identity(), drug_exp_prop(), drug_external_links(), drug_food_interactions(), drug_general_information(), drug_groups(), drug_interactions(), drug_intern_brand(), drug_manufacturers(), drug_mixtures(), drug_packagers(), drug_patents(), drug_pdb_entries(), drug_pharmacology(), drug_prices(), drug_products(), drug_reactions_enzymes(), drug_reactions(), drug_salts(), drug_sequences(), drug_snp_adverse_reactions(), drug_snp_effects(), drug_syn()
```

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## **Examples**

```
## Not run:
# the same parameters and usage will be applied for any parser
# return only the parsed tibble
run_all_parsers()
# will throw an error, as database_connection is NULL
run_all_parsers(save_table = TRUE)
# save in database in SQLite in memory database and return parsed tibble
sqlite_con <- DBI::dbConnect(RSQLite::SQLite())</pre>
run_all_parsers(save_table = TRUE, database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in current location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE)
# save in database, save parsed tibble as csv,
# if it does not exist in current location and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_table = TRUE, save_csv = TRUE,
database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in given location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE, csv_path = TRUE)
# save parsed tibble as csv if it does not exist in current location and
# return parsed tibble.
# if the csv exist override it and return it.
run_all_parsers(save_csv = TRUE, csv_path = TRUE, override = TRUE)
## End(Not run)
```

drug\_classification

Drug Classification parser

## **Description**

A description of the hierarchical chemical classification of the drug; imported from ClassyFire.

# Usage

```
drug_classification(
  save_table = FALSE,
  save_csv = FALSE,
  csv_path = ".",
```

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```
override_csv = FALSE,
database_connection = NULL
)
```

# **Arguments**

save\_table boolean, save table in database if true.

save\_csv boolean, save csv version of parsed tibble if true

csv\_path location to save csv files into it, default is current location, save\_csv must be

true

override\_csv override existing csv, if any, in case it is true in the new parse operation

database\_connection

DBI connection object that holds a connection to user defined database. If save\_table is enabled without providing value for this function an error will

be thrown.

#### Value

a tibble with 9 variables:

description

direct-parent

kingdom

superclass

class

subclass

alternative-parent One or more alternative parents

substituent One or more substituents

drugbank\_id drugbank id

## read\_drugbank\_xml\_db

read\_drugbank\_xml\_db function must be called first before any parser.

If read\_drugbank\_xml\_db is called before for any reason, so no need to call it again before calling this function.

#### See Also

```
Other drugs: drug_affected_organisms(), drug_ahfs_codes(), drug_atc_codes(), drug_calc_prop(), drug_categories(), drug_dosages(), drug_ex_identity(), drug_exp_prop(), drug_external_links(), drug_food_interactions(), drug_general_information(), drug_groups(), drug_interactions(), drug_intern_brand(), drug_manufacturers(), drug_mixtures(), drug_packagers(), drug_patents(), drug_pdb_entries(), drug_pharmacology(), drug_prices(), drug_products(), drug_reactions_enzymes(), drug_reactions(), drug_salts(), drug_sequences(), drug_snp_adverse_reactions(), drug_snp_effects(), drug_syn()
```

drug\_dosages

# **Examples**

```
## Not run:
# the same parameters and usage will be applied for any parser
# return only the parsed tibble
run_all_parsers()
# will throw an error, as database_connection is NULL
run_all_parsers(save_table = TRUE)
# save in database in SQLite in memory database and return parsed tibble
sqlite_con <- DBI::dbConnect(RSQLite::SQLite())</pre>
run_all_parsers(save_table = TRUE, database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in current location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE)
# save in database, save parsed tibble as csv,
# if it does not exist in current location and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_table = TRUE, save_csv = TRUE,
database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in given location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE, csv_path = TRUE)
# save parsed tibble as csv if it does not exist in current location and
# return parsed tibble.
# if the csv exist override it and return it.
run_all_parsers(save_csv = TRUE, csv_path = TRUE, override = TRUE)
## End(Not run)
```

drug\_dosages

Drug Dosages parser

## **Description**

A list of the commercially available dosages of the drug.

# Usage

```
drug_dosages(
  save_table = FALSE,
  save_csv = FALSE,
  csv_path = ".",
```

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```
override_csv = FALSE,
database_connection = NULL
)
```

# **Arguments**

save\_table boolean, save table in database if true.

save\_csv boolean, save csv version of parsed tibble if true

csv\_path location to save csv files into it, default is current location, save\_csv must be

true

override\_csv override existing csv, if any, in case it is true in the new parse operation

database\_connection

DBI connection object that holds a connection to user defined database. If save\_table is enabled without providing value for this function an error will

be thrown.

#### Value

a tibble with the following variables:

form The pharmaceutical formulation by which the drug is introduced into the body

**route** The path by which the drug or product is taken into the body.

strength The amount of active drug ingredient provided in the dosage

drugbank\_id drugbank id

### read drugbank xml db

read\_drugbank\_xml\_db function must be called first before any parser.

If read\_drugbank\_xml\_db is called before for any reason, so no need to call it again before calling this function.

#### See Also

```
Other drugs: drug_affected_organisms(), drug_ahfs_codes(), drug_atc_codes(), drug_calc_prop(), drug_categories(), drug_classification(), drug_ex_identity(), drug_exp_prop(), drug_external_links(), drug_food_interactions(), drug_general_information(), drug_groups(), drug_interactions(), drug_intern_brand(), drug_manufacturers(), drug_mixtures(), drug_packagers(), drug_patents(), drug_pdb_entries(), drug_pharmacology(), drug_prices(), drug_products(), drug_reactions_enzymes(), drug_reactions(), drug_salts(), drug_sequences(), drug_snp_adverse_reactions(), drug_snp_effects(), drug_syn()
```

```
## Not run:
# the same parameters and usage will be applied for any parser
# return only the parsed tibble
run_all_parsers()
```

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```
# will throw an error, as database_connection is NULL
run_all_parsers(save_table = TRUE)
# save in database in SQLite in memory database and return parsed tibble
sqlite_con <- DBI::dbConnect(RSQLite::SQLite())</pre>
run_all_parsers(save_table = TRUE, database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in current location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE)
# save in database, save parsed tibble as csv,
# if it does not exist in current location and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_table = TRUE, save_csv = TRUE,
database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in given location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE, csv_path = TRUE)
# save parsed tibble as csv if it does not exist in current location and
# return parsed tibble.
# if the csv exist override it and return it.
run_all_parsers(save_csv = TRUE, csv_path = TRUE, override = TRUE)
## End(Not run)
```

drug\_element

extracts the given drug elements and return data as list of tibbles.

# **Description**

drug\_element returns list of tibbles of drugs selected elements.

## Usage

```
drug_element(
   elements_options = c("all"),
   save_table = FALSE,
   save_csv = FALSE,
   csv_path = ".",
   override_csv = FALSE,
   database_connection = NULL
)
```

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## **Arguments**

elements\_options

list, options of elements to be parsed. default is "all"

save\_table boolean, save table in database if true.

save\_csv boolean, save csv version of parsed tibble if true

location to save csv files into it, default is current location, save\_csv must be csv\_path

true

override\_csv override existing csv, if any, in case it is true in the new parse operation

database\_connection

DBI connection object that holds a connection to user defined database. If save\_table is enabled without providing value for this function an error will

be thrown. @return list of selected drug elements tibbles

### **Details**

this functions extracts selected element of drug nodes in **DrugBank** xml database with the option to save it in a predefined database via passed database connection. it takes two optional arguments to save the returned tibble in the database save\_table and database\_connection. it must be called after read\_drugbank\_xml\_db function like any other parser function. if read\_drugbank\_xml\_db is called before for any reason, so no need to call it again before calling this function.

drug\_element\_options can be called to know the valid options for this method

#### See Also

Other common: drug\_element\_options(), run\_all\_parsers()

```
## Not run:
# return only the parsed tibble
drug_element()
# will throw an error, as database_connection is NULL
drug_element(save_table = TRUE)
# save parsed tibble as csv if it does not exist in current location and
# return parsed tibble.
# if the csv exist before read it and return its data.
drug_element(save_csv = TRUE)
sqlite_con <- DBI::dbConnect(RSQLite::SQLite())</pre>
drug_element(save_table = TRUE, database_connection = sqlite_con)
# save in database, save parsed tibble as csv if it does not
# exist in current location and return parsed tibble.
# if the csv exist before read it and return its data.
drug_element(save_table = TRUE, save_csv = TRUE,
database_connection = sqlite_con)
```

```
# save parsed tibble as csv if it does not exist in given location and
# return parsed tibble.
# if the csv exist before read it and return its data.
drug_element(save_csv = TRUE, csv_path = TRUE)

# save parsed tibble as csv if it does not exist in current
# location and return parsed tibble.
# if the csv exist override it and return it.
drug_element(save_csv = TRUE, csv_path = TRUE, override = TRUE)
drug_element(c("drug_ahfs_codes", "drug_carriers"), save_table = TRUE)
drug_element(save_table = FALSE)
drug_element(c("drug_ahfs_codes", "drug_carriers"))

## End(Not run)
```

drug\_element\_options returns drug\_element valid options.

# **Description**

returns drug\_element valid options.

# Usage

```
drug_element_options()
```

# Value

list of drug\_element valid options

## See Also

Other common: drug\_element(), run\_all\_parsers()

```
## Not run:
drug_element_options()
## End(Not run)
```

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arug_exp_prop Drug Experimental Properties parser	drug_exp_prop	Drug Experimental Properties parser
---	---------------	-------------------------------------

# **Description**

Drug properties that have been experimentally proven

# Usage

```
drug_exp_prop(
  save_table = FALSE,
  save_csv = FALSE,
  csv_path = ".",
  override_csv = FALSE,
  database_connection = NULL
)
```

## **Arguments**

save\_table boolean, save table in database if true.

save\_csv boolean, save csv version of parsed tibble if true

csv\_path location to save csv files into it, default is current location, save\_csv must be

true

override\_csv override existing csv, if any, in case it is true in the new parse operation

database\_connection

DBI connection object that holds a connection to user defined database. If save\_table is enabled without providing value for this function an error will

be thrown.

## Value

a tibble with the following variables:

kind Name of the property.

value Drug properties that have been experimentally proven.

**source** Reference to the source of this experimental data.

drugbank\_id drugbank id

The following experimental properties are provided:

Water Solubility The experimentally determined aqueous solubility of the molecule.

Molecular Formula Protein formula of Biotech drugs

Molecular Weight Protein weight of Biotech drugs.

**Melting Point** The experimentally determined temperature at which the drug molecule changes from solid to liquid at atmospheric temperature.

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**Boiling Point** The experimentally determined temperature at which the drug molecule changes from liquid to gas at atmospheric temperature.

**Hydrophobicity** The ability of a molecule to repel water rather than absorb or dissolve water.

**Isoelectric Point** The pH value at which the net electric charge of a molecule is zero.

caco2 Permeability A continuous line of heterogenous human epithelial colorectal adenocarcinoma cells, CAC02 cells are employed as a model of human intestinal absorption of various drugs and compounds. CAC02 cell permeability is ultimately an assay to measure drug absorption.

**pKa** The experimentally determined pka value of the molecule

**logP** The experimentally determined partition coefficient (LogP) based on the ratio of solubility of the molecule in 1-octanol compared to water.

**logS** The intrinsic solubility of a given compound is the concentration in equilibrium with its solid phase that dissolves into solution, given as the natural logarithm (LogS) of the concentration.

**Radioactivity** The property to spontaneously emit particles (alpha, beta, neutron) or radiation (gamma, K capture), or both at the same time, from the decay of certain nuclides.

### read drugbank xml db

read\_drugbank\_xml\_db function must be called first before any parser.

If read\_drugbank\_xml\_db is called before for any reason, so no need to call it again before calling this function.

#### See Also

```
Other drugs: drug_affected_organisms(), drug_ahfs_codes(), drug_atc_codes(), drug_calc_prop(), drug_categories(), drug_classification(), drug_dosages(), drug_ex_identity(), drug_external_links(), drug_food_interactions(), drug_general_information(), drug_groups(), drug_interactions(), drug_intern_brand(), drug_manufacturers(), drug_mixtures(), drug_packagers(), drug_patents(), drug_pdb_entries(), drug_pharmacology(), drug_prices(), drug_products(), drug_reactions_enzymes(), drug_reactions(), drug_salts(), drug_sequences(), drug_snp_adverse_reactions(), drug_snp_effects(), drug_syn()
```

```
## Not run:
# the same parameters and usage will be applied for any parser
# return only the parsed tibble
run_all_parsers()

# will throw an error, as database_connection is NULL
run_all_parsers(save_table = TRUE)

# save in database in SQLite in memory database and return parsed tibble
sqlite_con <- DBI::dbConnect(RSQLite::SQLite())
run_all_parsers(save_table = TRUE, database_connection = sqlite_con)

# save parsed tibble as csv if it does not exist in current location,
# and return parsed tibble.</pre>
```

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```
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE)
# save in database, save parsed tibble as csv,
# if it does not exist in current location and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_table = TRUE, save_csv = TRUE,
database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in given location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE, csv_path = TRUE)
# save parsed tibble as csv if it does not exist in current location and
# return parsed tibble.
# if the csv exist override it and return it.
run_all_parsers(save_csv = TRUE, csv_path = TRUE, override = TRUE)
## End(Not run)
```

drug\_external\_links

Drug External Links parser

## **Description**

Links to other websites or databases providing information about this drug.

### Usage

```
drug_external_links(
  save_table = FALSE,
  save_csv = FALSE,
  csv_path = ".",
  override_csv = FALSE,
  database_connection = NULL
)
```

# Arguments

save\_table boolean, save table in database if true.

save\_csv boolean, save csv version of parsed tibble if true

csv\_path location to save csv files into it, default is current location, save\_csv must be

true

override\_csv override existing csv, if any, in case it is true in the new parse operation

database\_connection

DBI connection object that holds a connection to user defined database. If save\_table is enabled without providing value for this function an error will be thrown.

#### Value

```
a tibble with the following variables:

resource Name of the source website.

identifier Identifier for this drug in the given resource drugbank_id drugbank id
```

# read\_drugbank\_xml\_db

```
read_drugbank_xml_db function must be called first before any parser.
```

If read\_drugbank\_xml\_db is called before for any reason, so no need to call it again before calling this function.

#### See Also

```
Other drugs: drug_affected_organisms(), drug_ahfs_codes(), drug_atc_codes(), drug_calc_prop(), drug_categories(), drug_classification(), drug_dosages(), drug_ex_identity(), drug_exp_prop(), drug_food_interactions(), drug_general_information(), drug_groups(), drug_interactions(), drug_intern_brand(), drug_manufacturers(), drug_mixtures(), drug_packagers(), drug_patents(), drug_pdb_entries(), drug_pharmacology(), drug_prices(), drug_products(), drug_reactions_enzymes(), drug_reactions(), drug_salts(), drug_sequences(), drug_snp_adverse_reactions(), drug_snp_effects(), drug_syn()
```

```
# the same parameters and usage will be applied for any parser
# return only the parsed tibble
run_all_parsers()
# will throw an error, as database_connection is NULL
run_all_parsers(save_table = TRUE)
# save in database in SQLite in memory database and return parsed tibble
sqlite_con <- DBI::dbConnect(RSQLite::SQLite())</pre>
run_all_parsers(save_table = TRUE, database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in current location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE)
# save in database, save parsed tibble as csv,
# if it does not exist in current location and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_table = TRUE, save_csv = TRUE,
database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in given location,
# and return parsed tibble.
```

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```
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE, csv_path = TRUE)

# save parsed tibble as csv if it does not exist in current location and
# return parsed tibble.
# if the csv exist override it and return it.
run_all_parsers(save_csv = TRUE, csv_path = TRUE, override = TRUE)
## End(Not run)
```

drug\_ex\_identity

Drug External Identifiers parser

# **Description**

Identifiers used in other websites or databases providing information about this drug.

# Usage

```
drug_ex_identity(
  save_table = FALSE,
  save_csv = FALSE,
  csv_path = ".",
  override_csv = FALSE,
  database_connection = NULL
)
```

#### Arguments

save\_table boolean, save table in database if true.

save\_csv boolean, save csv version of parsed tibble if true

csv\_path location to save csv files into it, default is current location, save\_csv must be

true

override\_csv override existing csv, if any, in case it is true in the new parse operation

database\_connection

DBI connection object that holds a connection to user defined database. If save\_table is enabled without providing value for this function an error will

be thrown.

# Value

a tibble with the following variables:

resource Name of the source database.

identifier Identifier for this drug in the given resource.

drugbank\_id drugbank id

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### read\_drugbank\_xml\_db

read\_drugbank\_xml\_db function must be called first before any parser.

If read\_drugbank\_xml\_db is called before for any reason, so no need to call it again before calling this function.

#### See Also

```
Other drugs: drug_affected_organisms(), drug_ahfs_codes(), drug_atc_codes(), drug_calc_prop(), drug_categories(), drug_classification(), drug_dosages(), drug_exp_prop(), drug_external_links(), drug_food_interactions(), drug_general_information(), drug_groups(), drug_interactions(), drug_intern_brand(), drug_manufacturers(), drug_mixtures(), drug_packagers(), drug_patents(), drug_pdb_entries(), drug_pharmacology(), drug_prices(), drug_products(), drug_reactions_enzymes(), drug_reactions(), drug_salts(), drug_sequences(), drug_snp_adverse_reactions(), drug_snp_effects(), drug_syn()
```

```
## Not run:
# the same parameters and usage will be applied for any parser
# return only the parsed tibble
run_all_parsers()
# will throw an error, as database_connection is NULL
run_all_parsers(save_table = TRUE)
# save in database in SQLite in memory database and return parsed tibble
sqlite_con <- DBI::dbConnect(RSQLite::SQLite())</pre>
run_all_parsers(save_table = TRUE, database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in current location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE)
# save in database, save parsed tibble as csv,
# if it does not exist in current location and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_table = TRUE, save_csv = TRUE,
database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in given location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE, csv_path = TRUE)
# save parsed tibble as csv if it does not exist in current location and
# return parsed tibble.
# if the csv exist override it and return it.
run_all_parsers(save_csv = TRUE, csv_path = TRUE, override = TRUE)
## End(Not run)
```

```
drug_food_interactions
```

Drug Groups parser

# **Description**

Food that may interact with this drug.

### Usage

```
drug_food_interactions(
   save_table = FALSE,
   save_csv = FALSE,
   csv_path = ".",
   override_csv = FALSE,
   database_connection = NULL
)
```

# **Arguments**

save\_table boolean, save table in database if true.

save\_csv boolean, save csv version of parsed tibble if true

csv\_path location to save csv files into it, default is current location, save\_csv must be

true

override\_csv override existing csv, if any, in case it is true in the new parse operation

database\_connection

DBI connection object that holds a connection to user defined database. If save\_table is enabled without providing value for this function an error will be thrown.

### Value

a tibble with the following variables:

## food-interaction

drugbank\_id drugbank id

## read\_drugbank\_xml\_db

read\_drugbank\_xml\_db function must be called first before any parser.

If read\_drugbank\_xml\_db is called before for any reason, so no need to call it again before calling this function.

#### See Also

```
Other drugs: drug_affected_organisms(), drug_ahfs_codes(), drug_atc_codes(), drug_calc_prop(), drug_categories(), drug_classification(), drug_dosages(), drug_ex_identity(), drug_exp_prop(), drug_external_links(), drug_general_information(), drug_groups(), drug_interactions(), drug_intern_brand(), drug_manufacturers(), drug_mixtures(), drug_packagers(), drug_patents(), drug_pdb_entries(), drug_pharmacology(), drug_prices(), drug_products(), drug_reactions_enzymes(), drug_reactions(), drug_salts(), drug_sequences(), drug_snp_adverse_reactions(), drug_snp_effects(), drug_syn()
```

### **Examples**

```
## Not run:
# the same parameters and usage will be applied for any parser
# return only the parsed tibble
run_all_parsers()
# will throw an error, as database_connection is NULL
run_all_parsers(save_table = TRUE)
# save in database in SQLite in memory database and return parsed tibble
sqlite_con <- DBI::dbConnect(RSQLite::SQLite())</pre>
run_all_parsers(save_table = TRUE, database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in current location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE)
# save in database, save parsed tibble as csv,
# if it does not exist in current location and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_table = TRUE, save_csv = TRUE,
database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in given location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE, csv_path = TRUE)
# save parsed tibble as csv if it does not exist in current location and
# return parsed tibble.
# if the csv exist override it and return it.
run_all_parsers(save_csv = TRUE, csv_path = TRUE, override = TRUE)
## End(Not run)
```

drug\_general\_information

Drugs General Information parser

# **Description**

A description of the hierarchical chemical classification of the drug; imported from ClassyFire.

### Usage

```
drug_general_information(
   save_table = FALSE,
   save_csv = FALSE,
   csv_path = ".",
   override_csv = FALSE,
   database_connection = NULL
)
```

## **Arguments**

save\_table boolean, save table in database if true.

save\_csv boolean, save csv version of parsed tibble if true

csv\_path location to save csv files into it, default is current location, save\_csv must be

true

override\_csv override existing csv, if any, in case it is true in the new parse operation

database\_connection

DBI connection object that holds a connection to user defined database. If save\_table is enabled without providing value for this function an error will be thrown.

# Value

a tibble with 15 variables:

primary\_key Drugbank id

other\_keys Other identifiers that may be associated with the drug

**type** Either small molecule, or biotech. Biotech is used for any drug that is derived from living systems or organisms, usually composed of high molecular weight mixtures of protein, while small molecule describes a low molecular weight organic compound.

#### name

created Date that this drug was first added to DrugBank.

updated Denotes when this drug was last updated in DrugBank.

description Descriptions of drug chemical properties, history and regulatory status.

**cas\_number** The Chemical Abstracts Service (CAS) registry number assigned to the drug.

unii Unique Ingredient Identifier (UNII) of this drug.

average\_mass The weighted average of the isotopic masses of the drug

state One of solid, liquid, or gas

monoisotopic\_mass The mass of the most abundant isotope of the drug

**synthesis\_reference** Citation for synthesis of the drug molecule.

**fda\_label** Contains a URL for accessing the uploaded United States Food and Drug Administration (FDA) Monograph for this drug.

msds Contains a URL for accessing the Material Safety Data Sheet (MSDS) for this drug.

## read\_drugbank\_xml\_db

read\_drugbank\_xml\_db function must be called first before any parser.

If read\_drugbank\_xml\_db is called before for any reason, so no need to call it again before calling this function.

#### See Also

```
Other drugs: drug_affected_organisms(), drug_ahfs_codes(), drug_atc_codes(), drug_calc_prop(), drug_categories(), drug_classification(), drug_dosages(), drug_ex_identity(), drug_exp_prop(), drug_external_links(), drug_food_interactions(), drug_groups(), drug_interactions(), drug_intern_brand(), drug_manufacturers(), drug_mixtures(), drug_packagers(), drug_patents(), drug_pdb_entries(), drug_pharmacology(), drug_prices(), drug_products(), drug_reactions_enzymes(), drug_reactions(), drug_salts(), drug_sequences(), drug_snp_adverse_reactions(), drug_snp_effects(), drug_syn()
```

```
## Not run:
# the same parameters and usage will be applied for any parser
# return only the parsed tibble
run_all_parsers()
# will throw an error, as database_connection is NULL
run_all_parsers(save_table = TRUE)
# save in database in SQLite in memory database and return parsed tibble
sqlite_con <- DBI::dbConnect(RSQLite::SQLite())</pre>
run_all_parsers(save_table = TRUE, database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in current location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE)
# save in database, save parsed tibble as csv,
# if it does not exist in current location and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_table = TRUE, save_csv = TRUE,
database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in given location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE, csv_path = TRUE)
# save parsed tibble as csv if it does not exist in current location and
```

drug\_groups 57

```
# return parsed tibble.
# if the csv exist override it and return it.
run_all_parsers(save_csv = TRUE, csv_path = TRUE, override = TRUE)
## End(Not run)
```

drug\_groups

Drug Groups parser

# **Description**

Groups that this drug belongs to. May include any of: approved, vet\_approved, nutraceutical, illicit, withdrawn, investigational, and experimental.

# Usage

```
drug_groups(
  save_table = FALSE,
  save_csv = FALSE,
  csv_path = ".",
  override_csv = FALSE,
  database_connection = NULL
)
```

# Arguments

save\_table boolean, save table in database if true.

save\_csv boolean, save csv version of parsed tibble if true

csv\_path location to save csv files into it, default is current location, save\_csv must be

true

override\_csv override existing csv, if any, in case it is true in the new parse operation

database\_connection

DBI connection object that holds a connection to user defined database. If save\_table is enabled without providing value for this function an error will be thrown.

### Value

```
a tibble with 2 variables:
```

### group

drugbank\_id drugbank id

## read\_drugbank\_xml\_db

read\_drugbank\_xml\_db function must be called first before any parser.

If read\_drugbank\_xml\_db is called before for any reason, so no need to call it again before calling this function.

58 drug\_interactions

#### See Also

Other drugs: drug\_affected\_organisms(), drug\_ahfs\_codes(), drug\_atc\_codes(), drug\_calc\_prop(), drug\_categories(), drug\_classification(), drug\_dosages(), drug\_ex\_identity(), drug\_exp\_prop(), drug\_external\_links(), drug\_food\_interactions(), drug\_general\_information(), drug\_interactions(), drug\_intern\_brand(), drug\_manufacturers(), drug\_mixtures(), drug\_packagers(), drug\_patents(), drug\_pdb\_entries(), drug\_pharmacology(), drug\_prices(), drug\_products(), drug\_reactions\_enzymes(), drug\_reactions(), drug\_salts(), drug\_sequences(), drug\_snp\_adverse\_reactions(), drug\_snp\_effects(), drug\_syn()

```
## Not run:
# the same parameters and usage will be applied for any parser
# return only the parsed tibble
run_all_parsers()
# will throw an error, as database_connection is NULL
run_all_parsers(save_table = TRUE)
# save in database in SQLite in memory database and return parsed tibble
sqlite_con <- DBI::dbConnect(RSQLite::SQLite())</pre>
run_all_parsers(save_table = TRUE, database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in current location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE)
# save in database, save parsed tibble as csv,
# if it does not exist in current location and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_table = TRUE, save_csv = TRUE,
database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in given location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE, csv_path = TRUE)
# save parsed tibble as csv if it does not exist in current location and
# return parsed tibble.
# if the csv exist override it and return it.
run_all_parsers(save_csv = TRUE, csv_path = TRUE, override = TRUE)
## End(Not run)
```

59 drug\_interactions

# **Description**

Drug-drug interactions detailing drugs that, when administered concomitantly with the drug of interest, will affect its activity or result in adverse effects. These interactions may be synergistic or antagonistic depending on the physiological effects and mechanism of action of each drug.

# **Usage**

```
drug_interactions(
  save_table = FALSE,
  save_csv = FALSE,
  csv_path = ".",
 override_csv = FALSE,
  database_connection = NULL
)
```

### **Arguments**

save table boolean, save table in database if true.

boolean, save csv version of parsed tibble if true save\_csv

csv\_path location to save csv files into it, default is current location, save\_csv must be

override\_csv override existing csv, if any, in case it is true in the new parse operation

database\_connection

DBI connection object that holds a connection to user defined database. If save\_table is enabled without providing value for this function an error will

be thrown.

# Value

a tibble with the following variables:

**drugbank-id** Drugbank ID of the interacting drug.

**name** Name of the interacting drug.

description Textual description of the physiological consequences of the drug interaction

drugbank\_id parent drugbank id

## read\_drugbank\_xml\_db

read\_drugbank\_xml\_db function must be called first before any parser.

If read\_drugbank\_xml\_db is called before for any reason, so no need to call it again before calling this function.

60 drug\_intern\_brand

#### See Also

```
Other drugs: drug_affected_organisms(), drug_ahfs_codes(), drug_atc_codes(), drug_calc_prop(), drug_categories(), drug_classification(), drug_dosages(), drug_ex_identity(), drug_exp_prop(), drug_external_links(), drug_food_interactions(), drug_general_information(), drug_groups(), drug_intern_brand(), drug_manufacturers(), drug_mixtures(), drug_packagers(), drug_patents(), drug_pdb_entries(), drug_pharmacology(), drug_prices(), drug_products(), drug_reactions_enzymes(), drug_reactions(), drug_salts(), drug_sequences(), drug_snp_adverse_reactions(), drug_snp_effects(), drug_syn()
```

```
## Not run:
# the same parameters and usage will be applied for any parser
# return only the parsed tibble
run_all_parsers()
# will throw an error, as database_connection is NULL
run_all_parsers(save_table = TRUE)
# save in database in SQLite in memory database and return parsed tibble
sqlite_con <- DBI::dbConnect(RSQLite::SQLite())</pre>
run_all_parsers(save_table = TRUE, database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in current location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE)
# save in database, save parsed tibble as csv,
# if it does not exist in current location and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_table = TRUE, save_csv = TRUE,
database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in given location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE, csv_path = TRUE)
# save parsed tibble as csv if it does not exist in current location and
# return parsed tibble.
# if the csv exist override it and return it.
run_all_parsers(save_csv = TRUE, csv_path = TRUE, override = TRUE)
## End(Not run)
```

drug\_intern\_brand 61

# **Description**

The proprietary names used by the manufacturers for commercially available forms of the drug, focusing on brand names for products that are available in countries other than Canada and the Unites States.

# Usage

```
drug_intern_brand(
  save_table = FALSE,
  save_csv = FALSE,
  csv_path = ".",
  override_csv = FALSE,
  database_connection = NULL
)
```

### **Arguments**

save\_table boolean, save table in database if true.

save\_csv boolean, save csv version of parsed tibble if true

csv\_path location to save csv files into it, default is current location, save\_csv must be

true

override\_csv override existing csv, if any, in case it is true in the new parse operation

database\_connection

DBI connection object that holds a connection to user defined database. If save\_table is enabled without providing value for this function an error will be thrown.

#### Value

a tibble with 4 variables:

brand The proprietary, well-known name for given to this drug by a manufacturer.

company The company or manufacturer that uses this name.

drugbank\_id drugbank id

### read\_drugbank\_xml\_db

read\_drugbank\_xml\_db function must be called first before any parser.

If read\_drugbank\_xml\_db is called before for any reason, so no need to call it again before calling this function.

## See Also

```
Other drugs: drug_affected_organisms(), drug_ahfs_codes(), drug_atc_codes(), drug_calc_prop(), drug_categories(), drug_classification(), drug_dosages(), drug_ex_identity(), drug_exp_prop(), drug_external_links(), drug_food_interactions(), drug_general_information(), drug_groups(), drug_interactions(), drug_manufacturers(), drug_mixtures(), drug_packagers(), drug_patents(),
```

62 drug\_manufacturers

```
drug_pdb_entries(), drug_pharmacology(), drug_prices(), drug_products(), drug_reactions_enzymes(),
drug_reactions(), drug_salts(), drug_sequences(), drug_snp_adverse_reactions(), drug_snp_effects(),
drug_syn()
```

## **Examples**

```
## Not run:
# the same parameters and usage will be applied for any parser
# return only the parsed tibble
run_all_parsers()
# will throw an error, as database_connection is NULL
run_all_parsers(save_table = TRUE)
# save in database in SQLite in memory database and return parsed tibble
sqlite_con <- DBI::dbConnect(RSQLite::SQLite())</pre>
run_all_parsers(save_table = TRUE, database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in current location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE)
# save in database, save parsed tibble as csv,
# if it does not exist in current location and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_table = TRUE, save_csv = TRUE,
database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in given location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE, csv_path = TRUE)
# save parsed tibble as csv if it does not exist in current location and
# return parsed tibble.
# if the csv exist override it and return it.
run_all_parsers(save_csv = TRUE, csv_path = TRUE, override = TRUE)
## End(Not run)
```

drug\_manufacturers

Drug Manufacturers parser

# Description

A list of companies that are manufacturing the commercially available forms of this drug that are available in Canada and the Unites States.

drug\_manufacturers 63

## Usage

```
drug_manufacturers(
   save_table = FALSE,
   save_csv = FALSE,
   csv_path = ".",
   override_csv = FALSE,
   database_connection = NULL
)
```

### **Arguments**

save\_table boolean, save table in database if true.

save\_csv boolean, save csv version of parsed tibble if true

csv\_path location to save csv files into it, default is current location, save\_csv must be

true

override\_csv override existing csv, if any, in case it is true in the new parse operation

database\_connection

DBI connection object that holds a connection to user defined database. If save\_table is enabled without providing value for this function an error will

be thrown.

#### Value

a tibble with the following variables:

generic A list of companies that are manufacturing the generic form of the drug.

url A link to the companies that are manufacturing the drug.

drugbank id drugbank id

## read\_drugbank\_xml\_db

read\_drugbank\_xml\_db function must be called first before any parser.

If read\_drugbank\_xml\_db is called before for any reason, so no need to call it again before calling this function.

### See Also

```
Other drugs: drug_affected_organisms(), drug_ahfs_codes(), drug_atc_codes(), drug_calc_prop(), drug_categories(), drug_classification(), drug_dosages(), drug_ex_identity(), drug_exp_prop(), drug_external_links(), drug_food_interactions(), drug_general_information(), drug_groups(), drug_interactions(), drug_intern_brand(), drug_mixtures(), drug_packagers(), drug_patents(), drug_pdb_entries(), drug_pharmacology(), drug_prices(), drug_products(), drug_reactions_enzymes(), drug_reactions(), drug_salts(), drug_sequences(), drug_snp_adverse_reactions(), drug_snp_effects(), drug_syn()
```

64 drug\_mixtures

## **Examples**

```
## Not run:
# the same parameters and usage will be applied for any parser
# return only the parsed tibble
run_all_parsers()
# will throw an error, as database_connection is NULL
run_all_parsers(save_table = TRUE)
# save in database in SQLite in memory database and return parsed tibble
sqlite_con <- DBI::dbConnect(RSQLite::SQLite())</pre>
run_all_parsers(save_table = TRUE, database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in current location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE)
# save in database, save parsed tibble as csv,
# if it does not exist in current location and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_table = TRUE, save_csv = TRUE,
database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in given location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE, csv_path = TRUE)
# save parsed tibble as csv if it does not exist in current location and
# return parsed tibble.
# if the csv exist override it and return it.
run_all_parsers(save_csv = TRUE, csv_path = TRUE, override = TRUE)
## End(Not run)
```

drug\_mixtures

Drug Mixtures parser

## **Description**

All commercially available products in which this drug is available in combination with other drug molecules

### **Usage**

```
drug_mixtures(
  save_table = FALSE,
  save_csv = FALSE,
```

drug\_mixtures 65

```
csv_path = ".",
override_csv = FALSE,
database_connection = NULL
)
```

## **Arguments**

save\_table boolean, save table in database if true.

save\_csv boolean, save csv version of parsed tibble if true

csv\_path location to save csv files into it, default is current location, save\_csv must be

true

override\_csv override existing csv, if any, in case it is true in the new parse operation

database\_connection

DBI connection object that holds a connection to user defined database. If save\_table is enabled without providing value for this function an error will be thrown.

#### Value

a tibble with 4 variables:

**name** The proprietary name provided by the manufacturer for this combination product.

**ingredients** A list of ingredients, separated by addition symbols

**supplemental-ingredients** List of additional active ingredients which are not clinically relevant to the main indication of the product, separated by addition symbols.

drugbank id drugbank id

#### read drugbank xml db

read\_drugbank\_xml\_db function must be called first before any parser.

If read\_drugbank\_xml\_db is called before for any reason, so no need to call it again before calling this function.

# See Also

```
Other drugs: drug_affected_organisms(), drug_ahfs_codes(), drug_atc_codes(), drug_calc_prop(), drug_categories(), drug_classification(), drug_dosages(), drug_ex_identity(), drug_exp_prop(), drug_external_links(), drug_food_interactions(), drug_general_information(), drug_groups(), drug_interactions(), drug_intern_brand(), drug_manufacturers(), drug_packagers(), drug_patents(), drug_pdb_entries(), drug_pharmacology(), drug_prices(), drug_products(), drug_reactions_enzymes(), drug_reactions(), drug_salts(), drug_sequences(), drug_snp_adverse_reactions(), drug_snp_effects(), drug_syn()
```

66 drug\_packagers

## **Examples**

```
## Not run:
# the same parameters and usage will be applied for any parser
# return only the parsed tibble
run_all_parsers()
# will throw an error, as database_connection is NULL
run_all_parsers(save_table = TRUE)
# save in database in SQLite in memory database and return parsed tibble
sqlite_con <- DBI::dbConnect(RSQLite::SQLite())</pre>
run_all_parsers(save_table = TRUE, database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in current location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE)
# save in database, save parsed tibble as csv,
# if it does not exist in current location and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_table = TRUE, save_csv = TRUE,
database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in given location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE, csv_path = TRUE)
# save parsed tibble as csv if it does not exist in current location and
# return parsed tibble.
# if the csv exist override it and return it.
run_all_parsers(save_csv = TRUE, csv_path = TRUE, override = TRUE)
## End(Not run)
```

drug\_packagers

Drug Packagers parser

## **Description**

A list of companies that are packaging the drug for re-distribution.

# Usage

```
drug_packagers(
   save_table = FALSE,
   save_csv = FALSE,
   csv_path = ".",
```

drug\_packagers 67

```
override_csv = FALSE,
database_connection = NULL
)
```

# **Arguments**

save\_table boolean, save table in database if true.

save\_csv boolean, save csv version of parsed tibble if true

csv\_path location to save csv files into it, default is current location, save\_csv must be

true

override\_csv override existing csv, if any, in case it is true in the new parse operation

database\_connection

DBI connection object that holds a connection to user defined database. If save\_table is enabled without providing value for this function an error will

be thrown.

#### Value

a tibble with 2 variables:

#### name

**url** A link to any companies that are packaging the drug for re-distribution.

drugbank\_id drugbank id

# read\_drugbank\_xml\_db

read\_drugbank\_xml\_db function must be called first before any parser.

If read\_drugbank\_xml\_db is called before for any reason, so no need to call it again before calling this function.

#### See Also

```
Other drugs: drug_affected_organisms(), drug_ahfs_codes(), drug_atc_codes(), drug_calc_prop(), drug_categories(), drug_classification(), drug_dosages(), drug_ex_identity(), drug_exp_prop(), drug_external_links(), drug_food_interactions(), drug_general_information(), drug_groups(), drug_interactions(), drug_intern_brand(), drug_manufacturers(), drug_mixtures(), drug_patents(), drug_pdb_entries(), drug_pharmacology(), drug_prices(), drug_products(), drug_reactions_enzymes(), drug_reactions(), drug_salts(), drug_sequences(), drug_snp_adverse_reactions(), drug_snp_effects(), drug_syn()
```

```
## Not run:
# the same parameters and usage will be applied for any parser
# return only the parsed tibble
run_all_parsers()
# will throw an error, as database_connection is NULL
```

68 drug\_patents

```
run_all_parsers(save_table = TRUE)
# save in database in SQLite in memory database and return parsed tibble
sqlite_con <- DBI::dbConnect(RSQLite::SQLite())</pre>
run_all_parsers(save_table = TRUE, database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in current location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE)
# save in database, save parsed tibble as csv,
# if it does not exist in current location and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_table = TRUE, save_csv = TRUE,
database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in given location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE, csv_path = TRUE)
# save parsed tibble as csv if it does not exist in current location and
# return parsed tibble.
# if the csv exist override it and return it.
run_all_parsers(save_csv = TRUE, csv_path = TRUE, override = TRUE)
## End(Not run)
```

drug\_patents

Drug Patents parser A property right issued by the United States Patent and Trademark Office (USPTO) to an inventor for a limited time, in exchange for public disclosure of the invention when the patent is granted. Drugs may be issued multiple patents.

## **Description**

Drug Patents parser A property right issued by the United States Patent and Trademark Office (USPTO) to an inventor for a limited time, in exchange for public disclosure of the invention when the patent is granted. Drugs may be issued multiple patents.

# Usage

```
drug_patents(
  save_table = FALSE,
  save_csv = FALSE,
  csv_path = ".",
  override_csv = FALSE,
  database_connection = NULL
)
```

drug\_patents 69

### **Arguments**

save\_table boolean, save table in database if true.

save\_csv boolean, save csv version of parsed tibble if true

csv\_path location to save csv files into it, default is current location, save csv must be

true

override\_csv override existing csv, if any, in case it is true in the new parse operation

database\_connection

DBI connection object that holds a connection to user defined database. If save\_table is enabled without providing value for this function an error will

be thrown.

## Value

a tibble with the following variables:

**number** The patent number(s) associated with the drug.

**country** The country that issued the patent rights.

approved The date that the patent request was filed.

**expires** The date that the patent rights expire.

pediatric-extension Indicates whether or not a pediatric extension has been approved for the patent.

Granted pediatric extensions provide an additional 6 months of market protection.

drugbank\_id drugbank id

## read\_drugbank\_xml\_db

read\_drugbank\_xml\_db function must be called first before any parser.

If read\_drugbank\_xml\_db is called before for any reason, so no need to call it again before calling this function.

# See Also

```
Other drugs: drug_affected_organisms(), drug_ahfs_codes(), drug_atc_codes(), drug_calc_prop(), drug_categories(), drug_classification(), drug_dosages(), drug_ex_identity(), drug_exp_prop(), drug_external_links(), drug_food_interactions(), drug_general_information(), drug_groups(), drug_interactions(), drug_intern_brand(), drug_manufacturers(), drug_mixtures(), drug_packagers(), drug_pdb_entries(), drug_pharmacology(), drug_prices(), drug_products(), drug_reactions_enzymes(), drug_reactions(), drug_salts(), drug_sequences(), drug_snp_adverse_reactions(), drug_snp_effects(), drug_syn()
```

```
## Not run:
# the same parameters and usage will be applied for any parser
# return only the parsed tibble
run_all_parsers()
# will throw an error, as database_connection is NULL
```

70 drug\_pathway

```
run_all_parsers(save_table = TRUE)
# save in database in SQLite in memory database and return parsed tibble
sqlite_con <- DBI::dbConnect(RSQLite::SQLite())</pre>
run_all_parsers(save_table = TRUE, database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in current location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE)
# save in database, save parsed tibble as csv,
# if it does not exist in current location and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_table = TRUE, save_csv = TRUE,
database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in given location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE, csv_path = TRUE)
# save parsed tibble as csv if it does not exist in current location and
# return parsed tibble.
# if the csv exist override it and return it.
run_all_parsers(save_csv = TRUE, csv_path = TRUE, override = TRUE)
## End(Not run)
```

drug\_pathway

Drug Pathway parser

# **Description**

Metabolic, disease, and biological pathways that the drug is involved in, as identified by the Small Molecule Protein Database (SMPDB).

# Usage

```
drug_pathway(
  save_table = FALSE,
  save_csv = FALSE,
  csv_path = ".",
  override_csv = FALSE,
  database_connection = NULL
)
```

drug\_pathway 71

# **Arguments**

save\_table boolean, save table in database if true.

save\_csv boolean, save csv version of parsed tibble if true

csv\_path location to save csv files into it, default is current location, save\_csv must be

true

override\_csv override existing csv, if any, in case it is true in the new parse operation

database\_connection

DBI connection object that holds a connection to user defined database. If save\_table is enabled without providing value for this function an error will

be thrown.

#### Value

a tibble with the following variables:

smpdb-id Small Molecule Pathway Database identifier for this pathway.

name Pathway name

category Pathway category

drugbank\_id drugbank id

# read\_drugbank\_xml\_db

read\_drugbank\_xml\_db function must be called first before any parser.

If read\_drugbank\_xml\_db is called before for any reason, so no need to call it again before calling this function.

#### See Also

```
Other pathway: drug_pathway_drugs(), drug_pathway_enzyme()
```

```
## Not run:
# the same parameters and usage will be applied for any parser
# return only the parsed tibble
run_all_parsers()

# will throw an error, as database_connection is NULL
run_all_parsers(save_table = TRUE)

# save in database in SQLite in memory database and return parsed tibble
sqlite_con <- DBI::dbConnect(RSQLite::SQLite())
run_all_parsers(save_table = TRUE, database_connection = sqlite_con)

# save parsed tibble as csv if it does not exist in current location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE)</pre>
```

72 drug\_pathway\_drugs

```
# save in database, save parsed tibble as csv,
# if it does not exist in current location and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_table = TRUE, save_csv = TRUE,
database_connection = sqlite_con)

# save parsed tibble as csv if it does not exist in given location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE, csv_path = TRUE)

# save parsed tibble as csv if it does not exist in current location and
# return parsed tibble.
# if the csv exist override it and return it.
run_all_parsers(save_csv = TRUE, csv_path = TRUE, override = TRUE)

## End(Not run)
```

drug\_pathway\_drugs

Drug Pathway Drugs parser

# **Description**

Drugs involved in this pathway.

# Usage

```
drug_pathway_drugs(
  save_table = FALSE,
  save_csv = FALSE,
  csv_path = ".",
  override_csv = FALSE,
  database_connection = NULL
)
```

# **Arguments**

save\_table boolean, save table in database if true.

save\_csv boolean, save csv version of parsed tibble if true

csv\_path location to save csv files into it, default is current location, save\_csv must be

true

override\_csv override existing csv, if any, in case it is true in the new parse operation

database\_connection

DBI connection object that holds a connection to user defined database. If save\_table is enabled without providing value for this function an error will be thrown.

drug\_pathway\_drugs 73

#### Value

a tibble with pathway drugsproperties

# read\_drugbank\_xml\_db

read\_drugbank\_xml\_db function must be called first before any parser.

If read\_drugbank\_xml\_db is called before for any reason, so no need to call it again before calling this function.

#### See Also

```
Other pathway: drug_pathway_enzyme(), drug_pathway()
```

```
## Not run:
# the same parameters and usage will be applied for any parser
# return only the parsed tibble
run_all_parsers()
# will throw an error, as database_connection is NULL
run_all_parsers(save_table = TRUE)
# save in database in SQLite in memory database and return parsed tibble
sqlite_con <- DBI::dbConnect(RSQLite::SQLite())</pre>
run_all_parsers(save_table = TRUE, database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in current location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE)
# save in database, save parsed tibble as csv,
# if it does not exist in current location and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_table = TRUE, save_csv = TRUE,
database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in given location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE, csv_path = TRUE)
# save parsed tibble as csv if it does not exist in current location and
# return parsed tibble.
# if the csv exist override it and return it.
run_all_parsers(save_csv = TRUE, csv_path = TRUE, override = TRUE)
## End(Not run)
```

drug\_pathway\_enzyme

Drug Pathway Enzymes parser

# Description

Enzymes involved in this pathway.

# Usage

```
drug_pathway_enzyme(
   save_table = FALSE,
   save_csv = FALSE,
   csv_path = ".",
   override_csv = FALSE,
   database_connection = NULL
)
```

# **Arguments**

save\_table boolean, save table in database if true.

save\_csv boolean, save csv version of parsed tibble if true

csv\_path location to save csv files into it, default is current location, save\_csv must be

true

override\_csv override existing csv, if any, in case it is true in the new parse operation

database\_connection

DBI connection object that holds a connection to user defined database. If save\_table is enabled without providing value for this function an error will be thrown.

# Value

a tibble with pathway properties

# read\_drugbank\_xml\_db

read\_drugbank\_xml\_db function must be called first before any parser.

If read\_drugbank\_xml\_db is called before for any reason, so no need to call it again before calling this function.

#### See Also

```
Other pathway: drug_pathway_drugs(), drug_pathway()
```

drug\_pdb\_entries 75

# **Examples**

```
## Not run:
# the same parameters and usage will be applied for any parser
# return only the parsed tibble
run_all_parsers()
# will throw an error, as database_connection is NULL
run_all_parsers(save_table = TRUE)
# save in database in SQLite in memory database and return parsed tibble
sqlite_con <- DBI::dbConnect(RSQLite::SQLite())</pre>
run_all_parsers(save_table = TRUE, database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in current location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE)
# save in database, save parsed tibble as csv,
# if it does not exist in current location and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_table = TRUE, save_csv = TRUE,
database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in given location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE, csv_path = TRUE)
# save parsed tibble as csv if it does not exist in current location and
# return parsed tibble.
# if the csv exist override it and return it.
run_all_parsers(save_csv = TRUE, csv_path = TRUE, override = TRUE)
## End(Not run)
```

drug\_pdb\_entries

Drug pdb-entries parser

# **Description**

Protein Data Bank (PDB) identifiers for this drug.

```
drug_pdb_entries(
  save_table = FALSE,
  save_csv = FALSE,
  csv_path = ".",
```

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```
override_csv = FALSE,
  database_connection = NULL
)
```

# **Arguments**

save\_table boolean, save table in database if true.

save\_csv boolean, save csv version of parsed tibble if true

csv\_path location to save csv files into it, default is current location, save\_csv must be

true

override\_csv override existing csv, if any, in case it is true in the new parse operation

database\_connection

DBI connection object that holds a connection to user defined database. If save\_table is enabled without providing value for this function an error will

be thrown.

#### Value

a tibble with the following variables:

```
pdb-entry
```

drugbank\_id drugbank id

#### read\_drugbank\_xml\_db

read\_drugbank\_xml\_db function must be called first before any parser.

If read\_drugbank\_xml\_db is called before for any reason, so no need to call it again before calling this function.

#### See Also

```
Other drugs: drug_affected_organisms(), drug_ahfs_codes(), drug_atc_codes(), drug_calc_prop(), drug_categories(), drug_classification(), drug_dosages(), drug_ex_identity(), drug_exp_prop(), drug_external_links(), drug_food_interactions(), drug_general_information(), drug_groups(), drug_interactions(), drug_intern_brand(), drug_manufacturers(), drug_mixtures(), drug_packagers(), drug_patents(), drug_pharmacology(), drug_prices(), drug_products(), drug_reactions_enzymes(), drug_reactions(), drug_salts(), drug_sequences(), drug_snp_adverse_reactions(), drug_snp_effects(), drug_syn()
```

```
## Not run:
# the same parameters and usage will be applied for any parser
# return only the parsed tibble
run_all_parsers()
# will throw an error, as database_connection is NULL
run_all_parsers(save_table = TRUE)
```

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```
# save in database in SQLite in memory database and return parsed tibble
sqlite_con <- DBI::dbConnect(RSQLite::SQLite())</pre>
run_all_parsers(save_table = TRUE, database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in current location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE)
# save in database, save parsed tibble as csv,
# if it does not exist in current location and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_table = TRUE, save_csv = TRUE,
database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in given location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE, csv_path = TRUE)
# save parsed tibble as csv if it does not exist in current location and
# return parsed tibble.
# if the csv exist override it and return it.
run_all_parsers(save_csv = TRUE, csv_path = TRUE, override = TRUE)
## End(Not run)
```

drug\_pharmacology

Drug Pharmacology parser

# Description

Describes the use, mechanism of action, pharmacokinetics, pharmacodynamics, and physiological or biochemical effects in the body.

# Usage

```
drug_pharmacology(
  save_table = FALSE,
  save_csv = FALSE,
  csv_path = ".",
  override_csv = FALSE,
  database_connection = NULL
)
```

# Arguments

```
save_table boolean, save table in database if true.

save_csv boolean, save csv version of parsed tibble if true
```

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csv\_path location to save csv files into it, default is current location, save\_csv must be

override\_csv override existing csv, if any, in case it is true in the new parse operation database\_connection

DBI connection object that holds a connection to user defined database. If save\_table is enabled without providing value for this function an error will be thrown

#### Value

a tibble with the following variables:

- **indication** The approved conditions, diseases, or states for which a drug can safely and effectively be used. An indication is considered to be FDA-approved when it has any of the following designations: NDA, ANDA, BLA, or OTC. May also include indications in other countries, such as Canada (through Health Canada) or in Europe (through the European Medicines Agency).
- pharmacodynamics A description of how the drug modifies or affects the organism it is being used in. May include effects in the body that are desired (enzyme or protein targets for example) and undesired (also known as "side effects"). This is in contrast to pharmacokinetics, which describes how the body modifies the drug being used.
- **mechanism\_of\_action** A component of pharmacodynamics that describes the biochemical interaction through which a drug produces its intended effect. May include the exact molecular protein or enzyme targets and/or a description of the physiological effects produced.
- **toxicity** Any adverse reaction, or side effect, that may or may not occur with use of the drug. May be attributed to a number of effects including: an enhanced therapeutic effect, rare anaphylactic reactions, interactions with other medications, or unanticipated binding of the molecule at different sites within the body.
- **metabolism** A description of the chemical degradation of the drug molecule within the body; most commonly by enzymes from the Cytochrome P450 (CYP) system in the liver.
- **absorption** A description of the movement of the drug from the site of administration into the bloodstream or target tissue. Common pharmacokinetic metrics used to evaluate absorption include Area Under the Curve (AUC), bioavailability (F), maximum concentration (Cmax), and time to maximum concentration (Tmax).
- half-life The period of time it takes for the amount of drug in the body to be reduced by one half. Provides a description of how quickly the drug is being eliminated and how much is available in the bloodstream.
- **protein-binding** A description of the drug's affinity for plama proteins and the proportion of the drug that is bound to them when in circulation within the body.
- route\_of\_elimination A description of the pathway that is used to excrete the drug from the body. Common pharmacokinetic parameters used to evaluate excretion include elemination half life, renal clearance, and tracking of radiolabelled compounds through the renal and GI system.
- **volume\_of\_distribution** The Vd of a drug represents the degree to which it is distributed into body tissue compared to the plasma.
- **clearance** A pharmacokinetic measurement of the rate of removal of the drug from plasma, expressed as mL/min; reflects the rate of elimination of the drug.

drugbank\_id drugbank id

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#### read\_drugbank\_xml\_db

read\_drugbank\_xml\_db function must be called first before any parser.

If read\_drugbank\_xml\_db is called before for any reason, so no need to call it again before calling this function.

#### See Also

```
Other drugs: drug_affected_organisms(), drug_ahfs_codes(), drug_atc_codes(), drug_calc_prop(), drug_categories(), drug_classification(), drug_dosages(), drug_ex_identity(), drug_exp_prop(), drug_external_links(), drug_food_interactions(), drug_general_information(), drug_groups(), drug_interactions(), drug_intern_brand(), drug_manufacturers(), drug_mixtures(), drug_packagers(), drug_patents(), drug_pdb_entries(), drug_prices(), drug_products(), drug_reactions_enzymes(), drug_reactions(), drug_salts(), drug_sequences(), drug_snp_adverse_reactions(), drug_snp_effects(), drug_syn()
```

```
## Not run:
# the same parameters and usage will be applied for any parser
# return only the parsed tibble
run_all_parsers()
# will throw an error, as database_connection is NULL
run_all_parsers(save_table = TRUE)
# save in database in SQLite in memory database and return parsed tibble
sqlite_con <- DBI::dbConnect(RSQLite::SQLite())</pre>
run_all_parsers(save_table = TRUE, database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in current location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE)
# save in database, save parsed tibble as csv,
# if it does not exist in current location and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_table = TRUE, save_csv = TRUE,
database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in given location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE, csv_path = TRUE)
# save parsed tibble as csv if it does not exist in current location and
# return parsed tibble.
# if the csv exist override it and return it.
run_all_parsers(save_csv = TRUE, csv_path = TRUE, override = TRUE)
## End(Not run)
```

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drug\_prices

Drug Prices Parsers

# **Description**

Unit drug prices

# Usage

```
drug_prices(
   save_table = FALSE,
   save_csv = FALSE,
   csv_path = ".",
   override_csv = FALSE,
   database_connection = NULL
)
```

# Arguments

save\_table boolean, save table in database if true.

save\_csv boolean, save csv version of parsed tibble if true

csv\_path location to save csv files into it, default is current location, save\_csv must be

true

override\_csv override existing csv, if any, in case it is true in the new parse operation

database\_connection

DBI connection object that holds a connection to user defined database. If save\_table is enabled without providing value for this function an error will be thrown.

# Value

```
a tibble with 5 variables:
```

# description

cost Drug price per unit

currency Currency of price, example: US.

unit

parent\_id drugbank id

# read\_drugbank\_xml\_db

read\_drugbank\_xml\_db function must be called first before any parser.

If read\_drugbank\_xml\_db is called before for any reason, so no need to call it again before calling this function.

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#### See Also

```
Other drugs: drug_affected_organisms(), drug_ahfs_codes(), drug_atc_codes(), drug_calc_prop(), drug_categories(), drug_classification(), drug_dosages(), drug_ex_identity(), drug_exp_prop(), drug_external_links(), drug_food_interactions(), drug_general_information(), drug_groups(), drug_interactions(), drug_intern_brand(), drug_manufacturers(), drug_mixtures(), drug_packagers(), drug_patents(), drug_pdb_entries(), drug_pharmacology(), drug_products(), drug_reactions_enzymes(), drug_reactions(), drug_salts(), drug_sequences(), drug_snp_adverse_reactions(), drug_snp_effects(), drug_syn()
```

```
## Not run:
# the same parameters and usage will be applied for any parser
# return only the parsed tibble
run_all_parsers()
# will throw an error, as database_connection is NULL
run_all_parsers(save_table = TRUE)
# save in database in SQLite in memory database and return parsed tibble
sqlite_con <- DBI::dbConnect(RSQLite::SQLite())</pre>
run_all_parsers(save_table = TRUE, database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in current location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE)
# save in database, save parsed tibble as csv,
# if it does not exist in current location and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_table = TRUE, save_csv = TRUE,
database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in given location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE, csv_path = TRUE)
# save parsed tibble as csv if it does not exist in current location and
# return parsed tibble.
# if the csv exist override it and return it.
run_all_parsers(save_csv = TRUE, csv_path = TRUE, override = TRUE)
## End(Not run)
```

82 drug\_products

# **Description**

A list of commercially available products in Canada and the United States that contain the drug.

# Usage

```
drug_products(
  save_table = FALSE,
  save_csv = FALSE,
  csv_path = ".",
  override_csv = FALSE,
  database_connection = NULL
)
```

# **Arguments**

save\_table boolean, save table in database if true.

save\_csv boolean, save csv version of parsed tibble if true

csv\_path location to save csv files into it, default is current location, save\_csv must be

true

override\_csv override existing csv, if any, in case it is true in the new parse operation

database\_connection

DBI connection object that holds a connection to user defined database. If save\_table is enabled without providing value for this function an error will be thrown.

#### Value

a tibble with 32 variables:

**name** The proprietary name(s) provided by the manufacturer for any commercially available products containing this drug.

**labeller** The corporation responsible for labelling this product.

ndc-id The National Drug Code (NDC) identifier of the drug

**ndc-product-code** The National Drug Code (NDC) product code from the FDA National Drug Code directory.

**dpd-id** Drug Product Database (DPD) identification number (a.k.a. DIN) from the Canadian Drug Product Database. Only present for drugs that are marketed in Canada

**ema-product-code** EMA product code from the European Medicines Agency Database. Only present for products that are authorised by central procedure for marketing in the European Union.

**ema-ma-number** EMA marketing authorisation number from the European Medicines Agency Database. Only present for products that are authorised by central procedure for marketing in the European Union.

started-marketing-on The starting date for market approval.

ended-marketing-on The ending date for market approval.

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**dosage-form** The pharmaceutical formulation by which the drug is introduced into the body.

strength The amount of active drug ingredient provided in the dosage

route The path by which the drug or product is taken into the body

**fda-application-number** The New Drug Application [NDA] number assigned to this drug by the FDA.

over-the-counter A list of Over The Counter (OTC) forms of the drug.

**generic** Whether this product is a generic drug.

**approved** Indicates whether this drug has been approved by the regulating government.

**country** The country where this commercially available drug has been approved.

**source** Source of this product information. For example, a value of DPD indicates this information was retrieved from the Canadian Drug Product Database.

**standing** One of good, discordant, or deprecated. Distinguishes products with up to date ingredient information (good) from products with conflicting information (discordant) or products that have been removed from an active label (deprecated).

standing-updated-on The date on which the standing was last updated

**standing-reason** Explains the non-good standing of the product. One of: ingredient\_change, code duplication, invalid, or removed.

jurisdiction-marketing-category The marketing category of this product in its jurisdiction

branded Whether this product has a named brand

prescription Whether this product is only available with a prescription

**unapproved** Whether this product is not approved in its jurisdiction

vaccine Whether this product is a vaccine

**allergenic** Whether this product is used in allergenic testing

**cosmetic** Whether this product is a cosmetic, such as sunscreen

kit Whether this product is a kit composed of multiple distinct parts

solo Whether this product has only a single active ingredient

available Whether this product can be sold in its jurisdiction

drugbank\_id drugbank id

# read\_drugbank\_xml\_db

read\_drugbank\_xml\_db function must be called first before any parser.

If read\_drugbank\_xml\_db is called before for any reason, so no need to call it again before calling this function.

#### See Also

```
Other drugs: drug_affected_organisms(), drug_ahfs_codes(), drug_atc_codes(), drug_calc_prop(), drug_categories(), drug_classification(), drug_dosages(), drug_ex_identity(), drug_exp_prop(), drug_external_links(), drug_food_interactions(), drug_general_information(), drug_groups(), drug_interactions(), drug_intern_brand(), drug_manufacturers(), drug_mixtures(), drug_packagers(), drug_patents(), drug_pdb_entries(), drug_pharmacology(), drug_prices(), drug_reactions_enzymes(), drug_reactions(), drug_salts(), drug_sequences(), drug_snp_adverse_reactions(), drug_snp_effects(), drug_syn()
```

84 drug\_reactions

# **Examples**

```
## Not run:
# the same parameters and usage will be applied for any parser
# return only the parsed tibble
run_all_parsers()
# will throw an error, as database_connection is NULL
run_all_parsers(save_table = TRUE)
# save in database in SQLite in memory database and return parsed tibble
sqlite_con <- DBI::dbConnect(RSQLite::SQLite())</pre>
run_all_parsers(save_table = TRUE, database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in current location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE)
# save in database, save parsed tibble as csv,
# if it does not exist in current location and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_table = TRUE, save_csv = TRUE,
database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in given location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE, csv_path = TRUE)
# save parsed tibble as csv if it does not exist in current location and
# return parsed tibble.
# if the csv exist override it and return it.
run_all_parsers(save_csv = TRUE, csv_path = TRUE, override = TRUE)
## End(Not run)
```

drug\_reactions

**Drug Reactions Parsers** 

# **Description**

Extract the sequential representation of the metabolic reactions that this drug molecule is involved in. Depending on available information, this may include metabolizing enzymes, reaction type, substrates, products, pharmacological activity of metabolites, and a structural representation of the biochemical reactions.

```
drug_reactions(
```

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```
save_table = FALSE,
save_csv = FALSE,
csv_path = ".",
override_csv = FALSE,
database_connection = NULL
)
```

# **Arguments**

save\_table boolean, save table in database if true.

save\_csv boolean, save csv version of parsed tibble if true

csv\_path location to save csv files into it, default is current location, save\_csv must be

true

override\_csv override existing csv, if any, in case it is true in the new parse operation

database\_connection

DBI connection object that holds a connection to user defined database. If save\_table is enabled without providing value for this function an error will

be thrown.

#### Value

a tibble with 5 variables:

sequence Reactions are displayed within a numerical sequence

**left\_drugbank\_name** The substrate of the reaction. Maybe a drug or a metabolite.

rightt\_drugbank\_name The product of the reaction. Maybe a drug or a metabolite.

left drugbank id

right\_drugbank\_id

parent\_id drugbank id

# read\_drugbank\_xml\_db

read\_drugbank\_xml\_db function must be called first before any parser.

If read\_drugbank\_xml\_db is called before for any reason, so no need to call it again before calling this function.

#### See Also

```
Other drugs: drug_affected_organisms(), drug_ahfs_codes(), drug_atc_codes(), drug_calc_prop(), drug_categories(), drug_classification(), drug_dosages(), drug_ex_identity(), drug_exp_prop(), drug_external_links(), drug_food_interactions(), drug_general_information(), drug_groups(), drug_interactions(), drug_intern_brand(), drug_manufacturers(), drug_mixtures(), drug_packagers(), drug_patents(), drug_pdb_entries(), drug_pharmacology(), drug_prices(), drug_products(), drug_reactions_enzymes(), drug_salts(), drug_sequences(), drug_snp_adverse_reactions(), drug_snp_effects(), drug_syn()
```

# **Examples**

```
## Not run:
 # the same parameters and usage will be applied for any parser
 # return only the parsed tibble
 run_all_parsers()
 # will throw an error, as database_connection is NULL
 run_all_parsers(save_table = TRUE)
 # save in database in SQLite in memory database and return parsed tibble
 sqlite_con <- DBI::dbConnect(RSQLite::SQLite())</pre>
 run_all_parsers(save_table = TRUE, database_connection = sqlite_con)
 # save parsed tibble as csv if it does not exist in current location,
 # and return parsed tibble.
 # if the csv exist before read it and return its data.
 run_all_parsers(save_csv = TRUE)
 # save in database, save parsed tibble as csv,
 # if it does not exist in current location and return parsed tibble.
 # if the csv exist before read it and return its data.
 run_all_parsers(save_table = TRUE, save_csv = TRUE,
 database_connection = sqlite_con)
 # save parsed tibble as csv if it does not exist in given location,
 # and return parsed tibble.
 # if the csv exist before read it and return its data.
 run_all_parsers(save_csv = TRUE, csv_path = TRUE)
 # save parsed tibble as csv if it does not exist in current location and
 # return parsed tibble.
 # if the csv exist override it and return it.
 run_all_parsers(save_csv = TRUE, csv_path = TRUE, override = TRUE)
 ## End(Not run)
drug_reactions_enzymes
```

ulug\_i eactions\_enzymes

Drug Reactions Enzymes Parsers

# **Description**

EEnzymes involved in metabolizing this drug

```
drug_reactions_enzymes(
  save_table = FALSE,
  save_csv = FALSE,
```

```
csv_path = ".",
override_csv = FALSE,
database_connection = NULL
)
```

#### **Arguments**

save\_table boolean, save table in database if true.

save\_csv boolean, save csv version of parsed tibble if true

csv\_path location to save csv files into it, default is current location, save\_csv must be

true

override\_csv override existing csv, if any, in case it is true in the new parse operation

database\_connection

DBI connection object that holds a connection to user defined database. If save\_table is enabled without providing value for this function an error will be thrown.

#### Value

a tibble with 3 variables:

name

uniprot-id

parent\_id drugbank id

# read\_drugbank\_xml\_db

read\_drugbank\_xml\_db function must be called first before any parser.

If read\_drugbank\_xml\_db is called before for any reason, so no need to call it again before calling this function.

## See Also

```
Other drugs: drug_affected_organisms(), drug_ahfs_codes(), drug_atc_codes(), drug_calc_prop(), drug_categories(), drug_classification(), drug_dosages(), drug_ex_identity(), drug_exp_prop(), drug_external_links(), drug_food_interactions(), drug_general_information(), drug_groups(), drug_interactions(), drug_intern_brand(), drug_manufacturers(), drug_mixtures(), drug_packagers(), drug_patents(), drug_pdb_entries(), drug_pharmacology(), drug_prices(), drug_products(), drug_reactions(), drug_salts(), drug_sequences(), drug_snp_adverse_reactions(), drug_snp_effects(), drug_syn()
```

```
## Not run:
# the same parameters and usage will be applied for any parser
# return only the parsed tibble
run_all_parsers()
```

88 drug\_salts

```
# will throw an error, as database_connection is NULL
run_all_parsers(save_table = TRUE)
# save in database in SQLite in memory database and return parsed tibble
sqlite_con <- DBI::dbConnect(RSQLite::SQLite())</pre>
run_all_parsers(save_table = TRUE, database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in current location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE)
# save in database, save parsed tibble as csv,
# if it does not exist in current location and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_table = TRUE, save_csv = TRUE,
database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in given location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE, csv_path = TRUE)
# save parsed tibble as csv if it does not exist in current location and
# return parsed tibble.
# if the csv exist override it and return it.
run_all_parsers(save_csv = TRUE, csv_path = TRUE, override = TRUE)
## End(Not run)
```

drug\_salts

Drug Salts parser

# **Description**

Available salt forms of the drug. Ions such as hydrochloride, sodium, and sulfate are often added to the drug molecule to increase solubility, dissolution, or absorption.

```
drug_salts(
   save_table = FALSE,
   save_csv = FALSE,
   csv_path = ".",
   override_csv = FALSE,
   database_connection = NULL
)
```

drug\_salts 89

#### **Arguments**

save\_table boolean, save table in database if true.

save\_csv boolean, save csv version of parsed tibble if true

csv\_path location to save csv files into it, default is current location, save\_csv must be

true

override\_csv override existing csv, if any, in case it is true in the new parse operation

database\_connection

DBI connection object that holds a connection to user defined database. If save\_table is enabled without providing value for this function an error will

be thrown.

#### Value

a tibble with 1 variables:

**drugbank-id** DrugBank identfiers of the available salt form(s).

**name** Name of the available salt form(s)

**unii** Unique Ingredient Identifier (UNII) of the available salt form(s).

**cas-number** Chemical Abstracts Service (CAS) registry number assigned to the salt form(s) of the drug.

inchikey IUPAC International Chemical Identifier (InChi) key identifier for the available salt form(s).

average-mass Average molecular mass: the weighted average of the isotopic masses of the salt.

monoisotopic-mass The mass of the most abundant isotope of the salt

**smiles** The simplified molecular-input line-entry system (SMILES) is a line notation used for describing the structure of chemical species using short ASCII strings; calculated by ChemAxon.

inchi A prediction of the IUPAC International Chemical Identifier (InChI); imported by ChemAxon.

**formula** Indicates the simple numbers of each type of atom within the molecule; calculated by ChemAxon.

drugbank\_id parent drugbank id

#### read\_drugbank\_xml\_db

read\_drugbank\_xml\_db function must be called first before any parser.

If read\_drugbank\_xml\_db is called before for any reason, so no need to call it again before calling this function.

# See Also

```
Other drugs: drug_affected_organisms(), drug_ahfs_codes(), drug_atc_codes(), drug_calc_prop(), drug_categories(), drug_classification(), drug_dosages(), drug_ex_identity(), drug_exp_prop(), drug_external_links(), drug_food_interactions(), drug_general_information(), drug_groups(), drug_interactions(), drug_intern_brand(), drug_manufacturers(), drug_mixtures(), drug_packagers(), drug_patents(), drug_pdb_entries(), drug_pharmacology(), drug_prices(), drug_products(), drug_reactions_enzymes(), drug_reactions(), drug_sequences(), drug_snp_adverse_reactions(), drug_snp_effects(), drug_syn()
```

90 drug\_sequences

# **Examples**

```
## Not run:
# the same parameters and usage will be applied for any parser
# return only the parsed tibble
run_all_parsers()
# will throw an error, as database_connection is NULL
run_all_parsers(save_table = TRUE)
# save in database in SQLite in memory database and return parsed tibble
sqlite_con <- DBI::dbConnect(RSQLite::SQLite())</pre>
run_all_parsers(save_table = TRUE, database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in current location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE)
# save in database, save parsed tibble as csv,
# if it does not exist in current location and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_table = TRUE, save_csv = TRUE,
database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in given location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE, csv_path = TRUE)
# save parsed tibble as csv if it does not exist in current location and
# return parsed tibble.
# if the csv exist override it and return it.
run_all_parsers(save_csv = TRUE, csv_path = TRUE, override = TRUE)
## End(Not run)
```

drug\_sequences

Drug Sequences parser

# **Description**

The amino acid sequence; provided if the drug is a peptide.

```
drug_sequences(
  save_table = FALSE,
  save_csv = FALSE,
  csv_path = ".",
```

drug\_sequences 91

```
override_csv = FALSE,
database_connection = NULL
)
```

## **Arguments**

save\_table boolean, save table in database if true.

save\_csv boolean, save csv version of parsed tibble if true

csv\_path location to save csv files into it, default is current location, save\_csv must be

true

override\_csv override existing csv, if any, in case it is true in the new parse operation

database\_connection

DBI connection object that holds a connection to user defined database. If save\_table is enabled without providing value for this function an error will

be thrown.

#### **Details**

Describes peptide sequences of biotech drugs

# Value

```
a tibble with the following variables:
```

```
sequence a textual representation of the sequence
```

format Currently, only the FASTA format is used

drugbank id drugbank id

#### read\_drugbank\_xml\_db

read\_drugbank\_xml\_db function must be called first before any parser.

If read\_drugbank\_xml\_db is called before for any reason, so no need to call it again before calling this function.

# See Also

```
Other drugs: drug_affected_organisms(), drug_ahfs_codes(), drug_atc_codes(), drug_calc_prop(), drug_categories(), drug_classification(), drug_dosages(), drug_ex_identity(), drug_exp_prop(), drug_external_links(), drug_food_interactions(), drug_general_information(), drug_groups(), drug_interactions(), drug_intern_brand(), drug_manufacturers(), drug_mixtures(), drug_packagers(), drug_patents(), drug_pdb_entries(), drug_pharmacology(), drug_prices(), drug_products(), drug_reactions_enzymes(), drug_reactions(), drug_salts(), drug_snp_adverse_reactions(), drug_snp_effects(), drug_syn()
```

# **Examples**

```
## Not run:
 # the same parameters and usage will be applied for any parser
 # return only the parsed tibble
 run_all_parsers()
 # will throw an error, as database_connection is NULL
 run_all_parsers(save_table = TRUE)
 # save in database in SQLite in memory database and return parsed tibble
 sqlite_con <- DBI::dbConnect(RSQLite::SQLite())</pre>
 run_all_parsers(save_table = TRUE, database_connection = sqlite_con)
 # save parsed tibble as csv if it does not exist in current location,
 # and return parsed tibble.
 # if the csv exist before read it and return its data.
 run_all_parsers(save_csv = TRUE)
 # save in database, save parsed tibble as csv,
 # if it does not exist in current location and return parsed tibble.
 # if the csv exist before read it and return its data.
 run_all_parsers(save_table = TRUE, save_csv = TRUE,
 database_connection = sqlite_con)
 # save parsed tibble as csv if it does not exist in given location,
 # and return parsed tibble.
 # if the csv exist before read it and return its data.
 run_all_parsers(save_csv = TRUE, csv_path = TRUE)
 # save parsed tibble as csv if it does not exist in current location and
 # return parsed tibble.
 # if the csv exist override it and return it.
 run_all_parsers(save_csv = TRUE, csv_path = TRUE, override = TRUE)
 ## End(Not run)
drug_snp_adverse_reactions
```

# Description

The adverse drug reactions that may occur as a result of the listed single nucleotide polymorphisms (SNPs)

Drug SNP Adverse Drug Reactions parser

```
drug_snp_adverse_reactions(
  save_table = FALSE,
```

```
save_csv = FALSE,
csv_path = ".",
override_csv = FALSE,
database_connection = NULL)
```

#### **Arguments**

save\_table boolean, save table in database if true.

save\_csv boolean, save csv version of parsed tibble if true

csv\_path location to save csv files into it, default is current location, save\_csv must be

true

override\_csv override existing csv, if any, in case it is true in the new parse operation

database\_connection

DBI connection object that holds a connection to user defined database. If save\_table is enabled without providing value for this function an error will

be thrown.

#### Value

a tibble with the following variables:

protein-name Proteins involved in this SNP.

gene-symbol Genes involved in this SNP.

uniprot-id Universal Protein Resource (UniProt) identifiers for proteins involved in this pathway.

**rs-id** The SNP Database identifier for this single nucleotide polymorphism.

allele The alleles associated with the identified SNP.

adverse-reaction

description

pubmed-id Reference to PubMed article.

drugbank\_id drugbank id

# read\_drugbank\_xml\_db

read\_drugbank\_xml\_db function must be called first before any parser.

If read\_drugbank\_xml\_db is called before for any reason, so no need to call it again before calling this function.

#### See Also

```
Other drugs: drug_affected_organisms(), drug_ahfs_codes(), drug_atc_codes(), drug_calc_prop(), drug_categories(), drug_classification(), drug_dosages(), drug_ex_identity(), drug_exp_prop(), drug_external_links(), drug_food_interactions(), drug_general_information(), drug_groups(), drug_interactions(), drug_intern_brand(), drug_manufacturers(), drug_mixtures(), drug_packagers(), drug_patents(), drug_pdb_entries(), drug_pharmacology(), drug_prices(), drug_products(), drug_reactions_enzymes(), drug_reactions(), drug_salts(), drug_sequences(), drug_snp_effects(), drug_syn()
```

94 drug\_snp\_effects

# **Examples**

```
## Not run:
# the same parameters and usage will be applied for any parser
# return only the parsed tibble
run_all_parsers()
# will throw an error, as database_connection is NULL
run_all_parsers(save_table = TRUE)
# save in database in SQLite in memory database and return parsed tibble
sqlite_con <- DBI::dbConnect(RSQLite::SQLite())</pre>
run_all_parsers(save_table = TRUE, database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in current location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE)
# save in database, save parsed tibble as csv,
# if it does not exist in current location and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_table = TRUE, save_csv = TRUE,
database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in given location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE, csv_path = TRUE)
# save parsed tibble as csv if it does not exist in current location and
# return parsed tibble.
# if the csv exist override it and return it.
run_all_parsers(save_csv = TRUE, csv_path = TRUE, override = TRUE)
## End(Not run)
```

drug\_snp\_effects

Drug SNP Effects parser

# **Description**

A list of single nucleotide polymorphisms (SNPs) relevent to drug activity or metabolism, and the effects these may have on pharmacological activity. SNP effects in the patient may require close monitoring, an increase or decrease in dose, or a change in therapy.

```
drug_snp_effects(
  save_table = FALSE,
```

drug\_snp\_effects 95

```
save_csv = FALSE,
  csv_path = ".",
  override_csv = FALSE,
  database_connection = NULL
)
```

# **Arguments**

save\_table boolean, save table in database if true.

save\_csv boolean, save csv version of parsed tibble if true

csv\_path location to save csv files into it, default is current location, save\_csv must be

true

override\_csv override existing csv, if any, in case it is true in the new parse operation

database\_connection

DBI connection object that holds a connection to user defined database. If save\_table is enabled without providing value for this function an error will

be thrown.

#### Value

a tibble with the following variables:

protein-name Proteins involved in this SNP.

gene-symbol Genes involved in this SNP.

uniprot-id Universal Protein Resource (UniProt) identifiers for proteins involved in this pathway.

**rs-id** The SNP Database identifier for this single nucleotide polymorphism.

allele The alleles associated with the identified SNP.

defining-change

**description** A written description of the SNP effects.

pubmed-id Reference to PubMed article.

drugbank\_id drugbank id

# read\_drugbank\_xml\_db

read\_drugbank\_xml\_db function must be called first before any parser.

If read\_drugbank\_xml\_db is called before for any reason, so no need to call it again before calling this function.

#### See Also

```
Other drugs: drug_affected_organisms(), drug_ahfs_codes(), drug_atc_codes(), drug_calc_prop(), drug_categories(), drug_classification(), drug_dosages(), drug_ex_identity(), drug_exp_prop(), drug_external_links(), drug_food_interactions(), drug_general_information(), drug_groups(), drug_interactions(), drug_intern_brand(), drug_manufacturers(), drug_mixtures(), drug_packagers(), drug_patents(), drug_pdb_entries(), drug_pharmacology(), drug_prices(), drug_products(), drug_reactions_enzymes(), drug_reactions(), drug_salts(), drug_sequences(), drug_snp_adverse_reactions() drug_syn()
```

96 drug\_syn

# **Examples**

```
## Not run:
# the same parameters and usage will be applied for any parser
# return only the parsed tibble
run_all_parsers()
# will throw an error, as database_connection is NULL
run_all_parsers(save_table = TRUE)
# save in database in SQLite in memory database and return parsed tibble
sqlite_con <- DBI::dbConnect(RSQLite::SQLite())</pre>
run_all_parsers(save_table = TRUE, database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in current location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE)
# save in database, save parsed tibble as csv,
# if it does not exist in current location and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_table = TRUE, save_csv = TRUE,
database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in given location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE, csv_path = TRUE)
# save parsed tibble as csv if it does not exist in current location and
# return parsed tibble.
# if the csv exist override it and return it.
run_all_parsers(save_csv = TRUE, csv_path = TRUE, override = TRUE)
## End(Not run)
```

drug\_syn

Drug Synonyms parser

# **Description**

Other names or identifiers that are associated with this drug.

```
drug_syn(
  save_table = FALSE,
  save_csv = FALSE,
  csv_path = ".",
```

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```
override_csv = FALSE,
database_connection = NULL
)
```

#### **Arguments**

save\_table boolean, save table in database if true.

save\_csv boolean, save csv version of parsed tibble if true

csv\_path location to save csv files into it, default is current location, save\_csv must be

true

override\_csv override existing csv, if any, in case it is true in the new parse operation

database\_connection

DBI connection object that holds a connection to user defined database. If save\_table is enabled without providing value for this function an error will be thrown.

# Value

a tibble with 3 variables:

language Names of the drug in languages other than English.

**coder** Organisation or source providing the synonym. For example, INN indicates the synonym is an International Nonproprietary Name, while IUPAC indicates the synonym is the nomenclature designated by the International Union of Pure and Applied Chemistry.

drugbank\_id drugbank id

# read\_drugbank\_xml\_db

read\_drugbank\_xml\_db function must be called first before any parser.

If read\_drugbank\_xml\_db is called before for any reason, so no need to call it again before calling this function.

#### See Also

```
Other drugs: drug_affected_organisms(), drug_ahfs_codes(), drug_atc_codes(), drug_calc_prop(), drug_categories(), drug_classification(), drug_dosages(), drug_ex_identity(), drug_exp_prop(), drug_external_links(), drug_food_interactions(), drug_general_information(), drug_groups(), drug_interactions(), drug_intern_brand(), drug_manufacturers(), drug_mixtures(), drug_packagers(), drug_patents(), drug_pdb_entries(), drug_pharmacology(), drug_prices(), drug_products(), drug_reactions_enzymes(), drug_reactions(), drug_salts(), drug_sequences(), drug_snp_adverse_reactions() drug_snp_effects()
```

```
## Not run:
# the same parameters and usage will be applied for any parser
# return only the parsed tibble
run_all_parsers()
```

```
# will throw an error, as database_connection is NULL
run_all_parsers(save_table = TRUE)
# save in database in SQLite in memory database and return parsed tibble
sqlite_con <- DBI::dbConnect(RSQLite::SQLite())</pre>
run_all_parsers(save_table = TRUE, database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in current location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE)
# save in database, save parsed tibble as csv,
# if it does not exist in current location and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_table = TRUE, save_csv = TRUE,
database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in given location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE, csv_path = TRUE)
# save parsed tibble as csv if it does not exist in current location and
# return parsed tibble.
# if the csv exist override it and return it.
run_all_parsers(save_csv = TRUE, csv_path = TRUE, override = TRUE)
## End(Not run)
```

get\_drugbank\_exported\_date

Return uploaded drugbank database exported date

# **Description**

get\_drugbank\_exported\_date returns uploaded drugbank database exported date.

#### Usage

```
get_drugbank_exported_date()
```

#### Value

drugbank exported date

get\_drugbank\_metadata 99

# **Examples**

```
## Not run:
get_drugbank_exported_date()
## End(Not run)
```

get\_drugbank\_metadata Return uploaded drugbank database metadata

# **Description**

get\_drugbank\_metadata returns uploaded drugbank database version and exported date.

# Usage

```
get_drugbank_metadata()
```

# Value

drugbank metadata

# **Examples**

```
## Not run:
get_drugbank_metadata()
## End(Not run)
```

get\_drugbank\_version Return uploaded drugbank database version

# **Description**

get\_drugbank\_version returns uploaded drugbank database version.

# Usage

```
get_drugbank_version()
```

# Value

drugbank version

```
## Not run:
get_drugbank_version()
## End(Not run)
```

links

links

Drugs/ Carriers/ Enzymes/ Targets/ Transporters links element parser

# **Description**

Return a list of websites that were used as references for Drugs/ Carriers/ Enzymes/ Targets/ Transporters

```
drugs_links(
  save_table = FALSE,
  save_csv = FALSE,
 csv_path = ".",
 override_csv = FALSE,
  database_connection = NULL
)
carriers_links(
  save_table = FALSE,
  save\_csv = FALSE,
  csv_path = ".",
  override_csv = FALSE,
  database\_connection = NULL
)
enzymes_links(
  save_table = FALSE,
  save_csv = FALSE,
  csv_path = ".",
  override_csv = FALSE,
  database_connection = NULL
)
targets_links(
  save_table = FALSE,
  save_csv = FALSE,
  csv_path = ".",
  override_csv = FALSE,
  database\_connection = NULL
)
transporters_links(
  save_table = FALSE,
  save_csv = FALSE,
  csv_path = ".",
  override_csv = FALSE,
```

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```
database_connection = NULL
)
```

# Arguments

save\_table boolean, save table in database if true.

save\_csv boolean, save csv version of parsed tibble if true

csv\_path location to save csv files into it, default is current location, save\_csv must be

true

override\_csv override existing csv, if any, in case it is true in the new parse operation

database\_connection

DBI connection object that holds a connection to user defined database. If save\_table is enabled without providing value for this function an error will

be thrown.

#### Value

a tibble with 4 variables:

ref-id Name of the source website

title Identifier for this drug in the given resource

url The url of the website

parent\_id drug/ carrier/ target/ enzyme/ transporter id

# read\_drugbank\_xml\_db

read\_drugbank\_xml\_db function must be called first before any parser.

If read\_drugbank\_xml\_db is called before for any reason, so no need to call it again before calling this function.

#### See Also

Other references: articles, attachments, books, references()

```
## Not run:
# the same parameters and usage will be applied for any parser
# return only the parsed tibble
run_all_parsers()

# will throw an error, as database_connection is NULL
run_all_parsers(save_table = TRUE)

# save in database in SQLite in memory database and return parsed tibble
sqlite_con <- DBI::dbConnect(RSQLite::SQLite())
run_all_parsers(save_table = TRUE, database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in current location,</pre>
```

```
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE)
# save in database, save parsed tibble as csv,
# if it does not exist in current location and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_table = TRUE, save_csv = TRUE,
database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in given location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE, csv_path = TRUE)
# save parsed tibble as csv if it does not exist in current location and
# return parsed tibble.
# if the csv exist override it and return it.
run_all_parsers(save_csv = TRUE, csv_path = TRUE, override = TRUE)
## End(Not run)
```

read\_drugbank\_xml\_db Reads **DrugBank** xml database and load it into memory.

# **Description**

read\_drugbank\_xml\_db loads **DrugBank** xml database full tree into memory.

# Usage

```
read_drugbank_xml_db(drugbank_db_path)
```

# **Arguments**

```
drugbank_db_path
```

string, full path for the DrugBank xml or zip file.

# **Details**

This functions reads **DrugBank** xml database and load it into memory for later processing. Hence; this method **must** be called before any other function in the package and it needs to be called one time only.

It takes one single mandatory argument which is the location of DrugBank db.

## Value

**TRUE** when the loading process into memory to be used by parser methods is completed successfully and **FALSE** otherwise.

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# **Examples**

```
## Not run:
read_drugbank_xml_db("db_full_path")
read_drugbank_xml_db(drugbank_db_path = "db_full_path")
## End(Not run)
```

references

Drugs/ Carriers/ Enzymes/ Targets/ Transporters references element parser

# Description

Return a list of all references for drugs, carriers, enzymes, targets or transporters

# Usage

```
references(
   save_table = FALSE,
   save_csv = FALSE,
   csv_path = ".",
   override_csv = FALSE,
   database_connection = NULL
)
```

# **Arguments**

save\_table boolean, save table in database if true.

save\_csv boolean, save csv version of parsed tibble if true

csv\_path location to save csv files into it, default is current location, save\_csv must be

true

override\_csv override existing csv, if any, in case it is true in the new parse operation

database\_connection

DBI connection object that holds a connection to user defined database. If save\_table is enabled without providing value for this function an error will be thrown.

#### read\_drugbank\_xml\_db

read\_drugbank\_xml\_db function must be called first before any parser.

If read\_drugbank\_xml\_db is called before for any reason, so no need to call it again before calling this function.

# See Also

Other references: articles, attachments, books, links

run\_all\_parsers

# **Examples**

```
## Not run:
# the same parameters and usage will be applied for any parser
# return only the parsed tibble
run_all_parsers()
# will throw an error, as database_connection is NULL
run_all_parsers(save_table = TRUE)
# save in database in SQLite in memory database and return parsed tibble
sqlite_con <- DBI::dbConnect(RSQLite::SQLite())</pre>
run_all_parsers(save_table = TRUE, database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in current location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE)
# save in database, save parsed tibble as csv,
# if it does not exist in current location and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_table = TRUE, save_csv = TRUE,
database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in given location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE, csv_path = TRUE)
# save parsed tibble as csv if it does not exist in current location and
# return parsed tibble.
# if the csv exist override it and return it.
run_all_parsers(save_csv = TRUE, csv_path = TRUE, override = TRUE)
## End(Not run)
```

run\_all\_parsers

extracts the all drug elements and return data as list of tibbles.

# **Description**

this functions extracts all element of drug nodes in **DrugBank** xml database with the option to save it in a predefined database via passed database connection. it takes two optional arguments to save the returned tibble in the database save\_table and database\_connection.

```
run_all_parsers(
   save_table = FALSE,
```

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```
save_csv = FALSE,
  csv_path = ".",
  override_csv = FALSE,
  database_connection = NULL
)
```

# **Arguments**

save\_table boolean, save table in database if true.

save\_csv boolean, save csv version of parsed tibble if true

csv\_path location to save csv files into it, default is current location, save\_csv must be

true

override\_csv override existing csv, if any, in case it is true in the new parse operation

database\_connection

DBI connection object that holds a connection to user defined database. If save\_table is enabled without providing value for this function an error will

be thrown.

# Value

all drug elements tibbles

# read\_drugbank\_xml\_db

read\_drugbank\_xml\_db function must be called first before any parser.

If read\_drugbank\_xml\_db is called before for any reason, so no need to call it again before calling this function.

#### See Also

```
Other common: drug_element_options(), drug_element()
Other collective_parsers: cett(), drugs()
```

```
## Not run:
# the same parameters and usage will be applied for any parser
# return only the parsed tibble
run_all_parsers()

# will throw an error, as database_connection is NULL
run_all_parsers(save_table = TRUE)

# save in database in SQLite in memory database and return parsed tibble
sqlite_con <- DBI::dbConnect(RSQLite::SQLite())
run_all_parsers(save_table = TRUE, database_connection = sqlite_con)

# save parsed tibble as csv if it does not exist in current location,
# and return parsed tibble.</pre>
```

run\_all\_parsers

```
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE)
# save in database, save parsed tibble as csv,
# if it does not exist in current location and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_table = TRUE, save_csv = TRUE,
database_connection = sqlite_con)
# save parsed tibble as csv if it does not exist in given location,
# and return parsed tibble.
# if the csv exist before read it and return its data.
run_all_parsers(save_csv = TRUE, csv_path = TRUE)
# save parsed tibble as csv if it does not exist in current location and
# return parsed tibble.
# if the csv exist override it and return it.
run_all_parsers(save_csv = TRUE, csv_path = TRUE, override = TRUE)
## End(Not run)
```

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