

Package ‘`covid19dbcand`’

August 26, 2020

Type Package

Title Selected 'Drugbank' Drugs for COVID-19 Treatment Related Data in R Format

Version 0.1.1

Depends R (>= 3.1)

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Description Provides different datasets parsed from 'Drugbank' <<https://www.drugbank.ca/covid-19>> database using 'dbparser' package. It is a smaller version from 'dbdataset' package. It contains only information about COVID-19 possible treatment.

License CC0

Encoding UTF-8

LazyData true

URL <https://github.com/MohammedFCIS/covid19dbcand>

BugReports <https://github.com/MohammedFCIS/covid19dbcand/issues>

Suggests knitr, rmarkdown, data.tree, DT, networkD3

VignetteBuilder knitr

RoxygenNote 7.1.0

NeedsCompilation no

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R topics documented:

actions	3
Affected_Organisms_Drug	4
AHFS_Codes_Drug	4
articles	5

ATC_Codes_Drug	6
attachments	6
books	7
Calculated_Properties_Drug	8
Categories_Drug	10
cett	10
Classifications_Drug	11
covid19dbcand	12
Dosages_Drug	13
Drugs	13
Drugs_Pathway_Drug	14
Enzymes_Pathway_Drug	15
Enzymes_Reactions_Drug	15
Experimental_Properties_Drug	16
External_Links_Drug	17
ext_id	17
Food_Interactions_Drug	19
go	20
Groups_Drug	21
Interactions_Drug	22
International_Brands_Drug	22
links	23
Manufacturers_Drug	24
Mixtures_Drug	25
Packagers_Drug	25
Patents_Drug	26
Pathways_Drug	27
PDB_Entries_Drug	27
pfam	28
Pharmacology	29
polypeptide	30
poly_syn	31
Prices_Drug	32
Products_Drug	33
Reactions_Drug	34
Salts_Drug	35
Sequences_Drug	36
SNP_Adverse_Drug_Reactions_Drug	36
SNP_Effects_Drug	37
Synonyms_Drug	38

actions	<i>Drug Carriers/ Enzymes/ Targets/ Transporters related Actions</i>
---------	--

Description

A collection of actions related to drugs carriers

Usage

Actions_Carrier_Drug

Actions_Enzyme_Drug

Actions_Target_Drug

Actions_Transporter_Drug

Format

a tibble with 2 variables:

text describe related action

parent_id drug/ carrier/ target/ enzyme/ transporter id

An object of class `spec_tbl_df` (inherits from `tbl_df`, `tbl`, `data.frame`) with 15 rows and 2 columns.

An object of class `spec_tbl_df` (inherits from `tbl_df`, `tbl`, `data.frame`) with 90 rows and 2 columns.

An object of class `spec_tbl_df` (inherits from `tbl_df`, `tbl`, `data.frame`) with 136 rows and 2 columns.

An object of class `spec_tbl_df` (inherits from `tbl_df`, `tbl`, `data.frame`) with 55 rows and 2 columns.

Source

[Drugbank Documentation](#)

Affected_Organisms_Drug

Drug related Affected Organisms

Description

A list of organisms in which the drug may display activity; activity may depend on local susceptibility patterns and resistance.

Usage

Affected_Organisms_Drug

Format

a tibble with 2 variables:

text affected organism description

parent_id drugbank id

Source

[Drugbank Documentation](#)

AHFS_Codes_Drug

The American Hospital Formulary Service (AHFS) identifier for Drugs

Description

A list of the American Hospital Formulary Service (AHFS) identifier for drugs

Usage

AHFS_Codes_Drug

Format

a tibble with 2 variables:

text ahfs code

parent_id drugbank id

Source

[Drugbank Documentation](#)

articles

Drugs/ Carriers/ Enzymes/ Targets/ Transporters related Articles

Description

A list of articles that were used as references for drugs carriers

Usage

Articles_Carrier_Drug

Articles_Drug

Articles_Enzyme_Drug

Articles_Target_Drug

Articles_Transporter_Drug

Format

a tibble with 4 variables:

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

pubmed-id The PubMed identifier for the article.

citation Article citation in a standard format.

parent_id drug/carrier/target/enzyme/transporter id

An object of class `spec_tbl_df` (inherits from `tbl_df`, `tbl`, `data.frame`) with 410 rows and 4 columns.

An object of class `spec_tbl_df` (inherits from `tbl_df`, `tbl`, `data.frame`) with 238 rows and 4 columns.

An object of class `spec_tbl_df` (inherits from `tbl_df`, `tbl`, `data.frame`) with 4003 rows and 4 columns.

An object of class `spec_tbl_df` (inherits from `tbl_df`, `tbl`, `data.frame`) with 1404 rows and 4 columns.

An object of class `spec_tbl_df` (inherits from `tbl_df`, `tbl`, `data.frame`) with 1312 rows and 4 columns.

Source

[Drugbank Documentation](#)

ATC_Codes_Drug	<i>Drug related ATC Codes</i>
----------------	-------------------------------

Description

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

Usage

ATC_Codes_Drug

Format

a tibble with 4 variables:

atc_code drug related atc code

level_n atc-code related level_n

code_n atc-code and level_n related code_n

drugbank-id drugbank id

Details

Each drug may have one or more atc-code.

Each atc-code has one or more level.

The atc-code and level elements each have a code which specifies the code assigned by [World Health Organization Anatomical Chemical Classification System](#).

Source

[Drugbank Documentation](#)

attachments	<i>Drugs/ Carriers/ Enzymes/ Targets/ Transporters Attachments</i>
-------------	--

Description

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

Usage

Attachments

Attachments_Enzymes

Attachments_Carriers

Attachments_Targets

Attachments_Transporters

Format

An object of class `spec_tbl_df` (inherits from `tbl_df`, `tbl`, `data.frame`) with 3 rows and 4 columns.

An object of class `tbl_df` (inherits from `tbl`, `data.frame`) with 388 rows and 4 columns.

An object of class `spec_tbl_df` (inherits from `tbl_df`, `tbl`, `data.frame`) with 6 rows and 4 columns.

An object of class `spec_tbl_df` (inherits from `tbl_df`, `tbl`, `data.frame`) with 11 rows and 4 columns.

An object of class `spec_tbl_df` (inherits from `tbl_df`, `tbl`, `data.frame`) with 37 rows and 4 columns.

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

Source

[Drugbank Documentation](#)

books

Drugs/ Carriers/ Enzymes/ Targets/ Transporters related Books

Description

A list of text books that were used as references for drugs

Usage

Books_Drug

Textbooks_Carrier_Drug

Textbooks_Enzyme_Drug

Textbooks_Target_Drug

Textbooks_Transporter_Drug

Format

a tibble with 4 variables:

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

isbn ISBN identifying the textbook.

citation A Textbook citation in a standard format.

parent_id drug/ carrier/ target/ enzyme/ transporter id

An object of class `spec_tbl_df` (inherits from `tbl_df`, `tbl`, `data.frame`) with 1 rows and 4 columns.

An object of class `spec_tbl_df` (inherits from `tbl_df`, `tbl`, `data.frame`) with 8 rows and 4 columns.

An object of class `spec_tbl_df` (inherits from `tbl_df`, `tbl`, `data.frame`) with 62 rows and 4 columns.

An object of class `spec_tbl_df` (inherits from `tbl_df`, `tbl`, `data.frame`) with 11 rows and 4 columns.

An object of class `spec_tbl_df` (inherits from `tbl_df`, `tbl`, `data.frame`) with 4 rows and 4 columns.

Source

[Drugbank Documentation](#)

Calculated_Properties_Drug

Drug Calculated Properties

Description

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

Usage

Calculated_Properties_Drug

Format

a tibble with 3 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

parent_key drugbank id

Details

Each drug may have one or more calculated property.

The following calculated properties are provided:

Property	Description
logP	The predicted partition coefficient (LogP) based on the ratio of solubility of the molecule in 1-octanol and water.
logS	The predicted solubility (LogS) of the molecule; predicted by ALOGPS .
IUPAC Name	The predicted International Union of Pure and Applied Chemistry (IUPAC) nomenclature for the molecule.
Traditional IUPAC Name	The non-systematic (or common) name for the molecule, which is not recognized by any formal nomenclature.
Molecular Weight	The predicted ratio of the average mass of one molecule of an element or compound to one twelfth of the mass of a carbon-12 atom.
Monoisotopic Weight	The predicted mass of the most abundant isotope of the drug; calculated by ChemAxon.
SMILES	The simplified molecular-input line-entry system (SMILES) is a line notation used for describing chemical structures.
InChI	A prediction of the IUPAC International Chemical Identifier (InChI); imported by ChemAxon.
InChIKey	The condensed digital representation of the IUPAC International Chemical Identifier (InChI); imported by ChemAxon.
Polar Surface Area (PSA)	A descriptor, based on the polarized atoms of the molecule, that allows estimation of transport properties.
Refractivity	The predicted molar refractivity of the molecule, which is strongly related to the volume of the molecule.
Polarizability	The predicted relative tendency of the electron cloud (charge distribution) of the molecule to be distorted by an external electric field.
Rotatable Bond Count	The predicted number of rotatable bonds in the molecule; predicted by ChemAxon. Unsaturated bonds are not counted.
H Bond Acceptor Count	A calculation of the sum of the hydrogen bond acceptor atoms. An acceptor atom always has a lone pair of electrons.
H Bond Donor Count	A calculation of the sum of the atoms in the molecule which have hydrogen bond donor property.
pKa (strongest acidic)	The strongest acidic pka value of the molecule; predicted by ChemAxon.
pKa (strongest basic)	The strongest basic pka value of the molecule; predicted by ChemAxon.
Physiological Charge	Charge of the molecule at physiological pH; predicted by ChemAxon.
Number of Rings	A calculation of the number of rings in the molecule; predicted by ChemAxon.
Bioavailability	Fraction of administered dose that is predicted to reach the systemic circulation; predicted by ChemAxon.
Rule of Five	A reflection of the absorption or permeation of a molecule; considered "yes" when the molecular weight is less than 500, the log P is less than 5, and the number of hydrogen bond donors and acceptors is less than 5.
Ghose Filter	A filter that defines drug-likeness constraints as follows: calculated log P is between -0.4 and 5.6, the number of hydrogen bond donors is less than 10, and the number of hydrogen bond acceptors is less than 10.
MDDR-Like Rule	Indicates compliance of drug-like characteristics based on number of rings, rigid bonds and rotatable bonds.

Source

[Drugbank Documentation](#)

Categories_Drug	<i>Drug Categories General categorizations of the drug</i>
-----------------	--

Description

Each drug may have one or more category.

Usage

Categories_Drug

Format

a tibble with 3 variables:

category Category name

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

parent_id drugbank id

Source

[Drugbank Documentation](#)

cett	<i>Carriers/ Enzymes/ Targets/ Transporters</i>
------	---

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.

Usage

Carriers_Drug

Enzymes_Drug

Targets_Drug

Transporters_Drug

Format

a tibble with 6 variables:

id 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.

position related position

parent_id drugbank id

An object of class `spec_tbl_df` (inherits from `tbl_df`, `tbl`, `data.frame`) with 15 rows and 6 columns.

An object of class `spec_tbl_df` (inherits from `tbl_df`, `tbl`, `data.frame`) with 90 rows and 8 columns.

An object of class `spec_tbl_df` (inherits from `tbl_df`, `tbl`, `data.frame`) with 59 rows and 6 columns.

An object of class `spec_tbl_df` (inherits from `tbl_df`, `tbl`, `data.frame`) with 49 rows and 6 columns.

Details

Each of targets, enzymes, carriers and transporters contain one or more child elements tibbles

Source

[Drugbank Documentation](#)

Classifications_Drug *Drug Classification*

Description

A description of the hierarchical chemical classification of the drug; imported from [ClassyFire](#).

Usage

Classifications_Drug

Format

a tibble with 9 variables:

description

direct_parent

kingdom

superclass

class

subclass

alternative_parents One or more alternative parents

substituents One or more substituents

drugbank_id drugbank id

Source

[Drugbank Documentation](#)

covid19dbcand

*covid19dbcand: A data package that contains different datasets extracted from **DrugBank** xml database.*

Description

The datasets in 'covid19dbcand' is related to [DrugBank](https://www.drugbank.ca/covid-19#drugs) selected drugs for covid-19

Details

The package is a smaller version from [dbdataset package](https://github.com/MohammedFCIS/dbdataset).

It is extracted using [dbparser](https://docs.ropensci.org/dbparser/)

For more information kindly check the reference/index (https://mohammedfcis.github.io/covid19dbcand/reference/index.htm)

 Dosages_Drug

Drug Dosages A list of the commercially available dosages of the drug.

Description

Each drug may have one or more dosage.

Usage

Dosages_Drug

Format

a tibble with 4 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

parent_id drugbank id

Source

[Drugbank Documentation](#)

 Drugs

Drugs

Description

Substance other than water and food that when administered by any route can cause a physiological or biological change in the body.

Usage

Drugs

Format

An object of class `tbl_df` (inherits from `tbl`, `data.frame`) with 33 rows and 15 columns.

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.

Source

[Drugbank Documentation](#)

Drugs_Pathway_Drug	<i>Pathway Drugs Pathway Drugs Each drug may have one or more pathway and vise versa</i>
--------------------	--

Description

Pathway Drugs Pathway Drugs Each drug may have one or more pathway and vise versa

Usage

Drugs_Pathway_Drug

Format

a tibble with 3 variables:

drugbank-id

name drug name

parent_id pathway id

Source

[Drugbank Documentation](#)

Enzymes_Pathway_Drug *Pathway Enzymes Enzymes involved in this pathway.*

Description

Each drug may have one or more pathway

Usage

Enzymes_Pathway_Drug

Format

a tibble with 2 variables:

text uniprot id

parent_id pathway id

Source

[Drugbank Documentation](#)

Enzymes_Reactions_Drug
Drug Reactions Enzymes Enzymes involved in metabolizing this drug.

Description

Drug Reactions Enzymes Enzymes involved in metabolizing this drug.

Usage

Enzymes_Reactions_Drug

Format

a tibble with 3 variables:

drugbank-id

name

uniprot-id uniprot id

Source

[Drugbank Documentation](#)

Experimental_Properties_Drug
Drug Experimental Properties

Description

Drug properties that have been experimentally proven. Each drug may have one or more experimental property.

Usage

Experimental_Properties_Drug

Format

a tibble with 4 variables:

kind Name of the property

value Drug properties that have been experimentally proven

source Reference to the source of this experimental data

parent_key drugbank key

Details

The following experimental properties are provided:

Property	Description
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 a
Boiling Point	The experimentally determined temperature at which the drug molecule changes from liquid to gas at a
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 heterogeneous human epithelial colorectal adenocarcinoma cells, CAC02 cells are
pKa	The experimentally determined pka value of the molecule.
logP	The experimentally determined partition coefficient (LogP) based on the ratio of solubility of the molecu
logS	The intrinsic solubility of a given compound is the concentration in equilibrium with its solid phase that
Radioactivity	The property to spontaneously emit particles (alpha, beta, neutron) or radiation (gamma, K capture), or l

Source

[Drugbank Documentation](#)

External_Links_Drug *Drugs External Links.*

Description

Each drug may have one or more link.

Usage

External_Links_Drug

Format

a tibble with 3 variables:

resource Name of the source website.

identifier Identifier for this drug in the given resource

parent_id drugbank id

Details

Links may be provided for the following resources:

- [RxList](#)
- [PDRhealth](#)
- [Drugs.com](#)

Source

[Drugbank Documentation](#)

ext_id *External Identifiers for Drugs/ Carriers/ Enzymes/ Targets/ Trans-
porters*

Description

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

Usage

External_Identifiers_Drug
External_Identifiers_Polypeptide_Carrier_Drug
External_Identifiers_Polypeptide_Enzyme_Drug
External_Identifiers_Polypeptide_Target_Drug
External_Identifiers_Transporter_Drug

Format

a tibble with following features:

resource Name of the source database
identifier Identifier for this drug in the given resource
parent_key drugbank key

An object of class `spec_tbl_df` (inherits from `tbl_df`, `tbl`, `data.frame`) with 232 rows and 3 columns.

An object of class `spec_tbl_df` (inherits from `tbl_df`, `tbl`, `data.frame`) with 0 rows and 3 columns.

An object of class `spec_tbl_df` (inherits from `tbl_df`, `tbl`, `data.frame`) with 0 rows and 3 columns.

An object of class `spec_tbl_df` (inherits from `tbl_df`, `tbl`, `data.frame`) with 0 rows and 3 columns.

An object of class `spec_tbl_df` (inherits from `tbl_df`, `tbl`, `data.frame`) with 0 rows and 3 columns.

Details

Each drug may have one or more external identifier.

Drug identifiers may be provided for the following resources

- [Wikipedia](#)
- [ChEBI](#)
- [ChEMBL](#)
- [PubChem Compound](#)
- [PubChem Substance](#)
- [Drugs Product Database \(DPD\)](#)
- [KEGG Compound](#)
- [KEGG Compound](#)
- [KEGG Drug](#)

- ChemSpider
- [BindingDB](#)
- [National Drug Code Directory](#)
- [GenBank](#)
- PharmGKB
- [PDB](#)
- [Guide to Pharmacology](#)
- ZINC
- [RxCUI](#)

Source

[Drugbank Documentation](#)

Food_Interactions_Drug

Drug Food Interactions

Description

Description of interactions this drug has with food.

Usage

Food_Interactions_Drug

Format

a tibble 2 variables:

interaction descripts of interactions this drug has with food.

parent_key drugbank key

Details

Each drug may have one or more food interaction.

Source

[Drugbank Documentation](#)

go *Carriers/ Enzymes/ Targets/ Transporters related Gene Ontology (GO)*

Description

The **Gene Ontology (GO)** Consortium identifier

Usage

GO_Classifiers_Polypeptide_Carrier_Drug

GO_Classifiers_Polypeptides_Enzyme_Drug

GO_Classifiers_Polypeptide_Target_Drug

GO_Classifiers_Polypeptide_Transporter_Drug

Format

a tibble with 3 variables:

category

description

polypeptide_id polypeptide id

An object of class `spec_tbl_df` (inherits from `tbl_df`, `tbl`, `data.frame`) with 0 rows and 3 columns.

An object of class `spec_tbl_df` (inherits from `tbl_df`, `tbl`, `data.frame`) with 0 rows and 3 columns.

An object of class `spec_tbl_df` (inherits from `tbl_df`, `tbl`, `data.frame`) with 0 rows and 3 columns.

An object of class `spec_tbl_df` (inherits from `tbl_df`, `tbl`, `data.frame`) with 0 rows and 3 columns.

Details

Each Carriers/ Enzymes/ Targets/ may have zero or more GO.

Source

[Drugbank Documentation](#)

Groups_Drug

Drug Groups

Description

Groups that this drug belongs to.

Usage

Groups_Drug

Format

a tibble with 2 variables:

group one of the above values

drugbank-id drugbank id

Details

Each drug may have one or more category.

Groups include:

- approved
- vet_approved
- nutraceutical
- illicit
- withdrawn
- investigational
- experimental

Source

[Drugbank Documentation](#)

Interactions_Drug #' Drug Interactions

Description

Describe interactions between the drug being described by the parent drug, and other drugs.

Usage

Interactions_Drug

Format

a tibble with 4 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

parent_key parent drugbank id

Details

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.

Each drug may have one or more drug interaction.

Source

[Drugbank Documentation](#)

International_Brands_Drug
Drug International Brands

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 United States.

Usage

International_Brands_Drug

Format

a tibble with 3 variables:

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

company The company or manufacturer that uses this name.

parent_key drugbank id

Details

Each drug may have one or more international brand.

Source

[Drugbank Documentation](#)

links	<i>Drugs/ Carriers/ Enzymes/ Targets/ Transporters related Links</i>
-------	--

Description

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

Usage

Links_Drug

Links_Carrier_Drug

Links_Enzyme_Drug

Links_Target_Drug

Links_Transporter_Drug

Format

a tibble with 3 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

An object of class `spec_tbl_df` (inherits from `tbl_df`, `tbl`, `data.frame`) with 94 rows and 4 columns.

An object of class `spec_tbl_df` (inherits from `tbl_df`, `tbl`, `data.frame`) with 88 rows and 4 columns.

An object of class `tbl_df` (inherits from `tbl`, `data.frame`) with 645 rows and 4 columns.

An object of class `spec_tbl_df` (inherits from `tbl_df`, `tbl`, `data.frame`) with 60 rows and 4 columns.

An object of class `spec_tbl_df` (inherits from `tbl_df`, `tbl`, `data.frame`) with 168 rows and 4 columns.

Details

Each drug/ carrier/ target/ enzyme/ transporter may have one or more link.

Source

[Drugbank Documentation](#)

Manufacturers_Drug *Drug Manufacturers*

Description

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

Usage

Manufacturers_Drug

Format

a tibble with 3 variables:

text the name or description of the manufacturer

parent_key drugbank id

Details

Each drug may have one or more Manufacturer.

Source

[Drugbank Documentation](#)

Mixtures_Drug	<i>Drug Mixture</i>
---------------	---------------------

Description

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

Usage

Mixtures_Drug

Format

a tibble with 3 variables:

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

ingredients A list of ingredients, separated by addition symbols.

parent_key drugbank id

Details

Each drug may have one or more mixture.

Source

[Drugbank Documentation](#)

Packagers_Drug	<i>Drug Packagers</i>
----------------	-----------------------

Description

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

Usage

Packagers_Drug

Format

a tibble with 3 variables:

name

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

parent_key drugbank id

Details

Each drug may have one or more Packagers.

Source

[Drugbank Documentation](#)

Patents_Drug

Drug Patent

Description

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

Patents_Drug

Format

a tibble with 6 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

parent_key drugbank id

Details

Each drug may have one or more patent.

Source

[Drugbank Documentation](#)

Pathways_Drug	<i>Drug Pathways</i>
---------------	----------------------

Description

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

Usage

Pathways_Drug

Format

a tibble with 4 variables:

smpdb_id [Small Molecule Protein Database \(SMPDB\)](#) identifier for this pathway.

name Pathway name

category Pathway category

parent_key drugbank id

Details

Each drug may have one or more pathway.

Source

[Drugbank Documentation](#)

PDB_Entries_Drug	<i>Drug PDB Entries</i>
------------------	-------------------------

Description

Protein Data Bank (PDB) identifiers for this drug

Usage

PDB_Entries_Drug

Format

a tibble with 2 variables:

text PDB identifier

parent_key drugbank id

Details

Each drug may have one or more PDB Entry

Source

[Drugbank Documentation](#)

pfam

PFAMs

Description

The [protein family \(pfam\)](#) identifier

Usage

PFAMS_Polypeptide_Carrier_Drug

PFAMS_Polypeptides_Enzyme_Drug

PFAMS_Polypeptide_Target_Drug

PFAMS_Polypeptid_Transporter_Drug

Format

a tibble with 3 variables:

identifier

name

polypeptide_id polypeptide id

An object of class spec_tbl_df (inherits from tbl_df, tbl, data.frame) with 0 rows and 3 columns.

An object of class spec_tbl_df (inherits from tbl_df, tbl, data.frame) with 0 rows and 3 columns.

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Details

Each Polypeptid may have one or more PFAM.

Source

[Drugbank Documentation](#)

Pharmacology

Drug Pharmacology

Description

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

Usage

Pharmacology

Format

An object of class `tbl_df` (inherits from `tbl`, `data.frame`) with 33 rows and 12 columns.

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 (C_{max}), and time to maximum concentration (T_{max}).

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 plasma 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 elimination 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

Source

[Drugbank Documentation](#)

polypeptide

Polypeptide

Description

Descriptions of identified polypeptide targets, enzymes, carriers, or transporters.

Usage

Polypeptides_Carrier_Drug

Polypeptides_Enzyme_Drug

Polypeptide_Target_Drug

Polypeptides_Transporter_Drug

Format

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.

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 drugbank id

An object of class spec_tbl_df (inherits from tbl_df, tbl, data.frame) with 3 rows and 20 columns.

An object of class spec_tbl_df (inherits from tbl_df, tbl, data.frame) with 35 rows and 20 columns.

An object of class spec_tbl_df (inherits from tbl_df, tbl, data.frame) with 50 rows and 20 columns.

An object of class spec_tbl_df (inherits from tbl_df, tbl, data.frame) with 17 rows and 20 columns.

Details

Each target, enzyme, carrier and transporter elements may include one or more polypeptide.

Source

[Drugbank Documentation](#)

poly_syn

Polypeptide Synonyms

Description

Alternate names or identifiers that may be associated with this polypeptide

Usage

Synonyms_Polypeptide_Carrier_Drug

Synonyms_Polypeptides_Enzyme_Drug

Synonyms_Polypeptide_Target_Drug

Synonyms_Polypeptide_Transporter_Drug

Format

a tibble with 2 variables:

syn alternative name

polypeptide_id polypeptide id

An object of class `spec_tbl_df` (inherits from `tbl_df`, `tbl`, `data.frame`) with 0 rows and 2 columns.

An object of class `spec_tbl_df` (inherits from `tbl_df`, `tbl`, `data.frame`) with 0 rows and 2 columns.

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Details

Each element may have one or more synonyms.

Source

[Drugbank Documentation](#)

Prices_Drug

Drug Prices

Description

Unit drug prices

Usage

Prices_Drug

Format

a tibble with 5 variables:

description

cost Drug price per unit

unit

currency Currency of price, example: USD

parent_key drugbank id

Details

Each drug may have one or more price

Source

[Drugbank Documentation](#)

Products_Drug

Drug Products

Description

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

Usage

Products_Drug

Format

a tibble with 19 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.

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.
parent_key drugbank id

Details

Each drug may have one or more product.

Source

[Drugbank Documentation](#)

Reactions_Drug	<i>Drug Reactions</i>
----------------	-----------------------

Description

A 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.

Usage

Reactions_Drug

Format

a tibble with 6 variables:

sequence Reactions are displayed within a numerical sequence.
left_drugbank_id The substrate of the reaction. May be a drug or a metabolite.
left_drugbank_name
right_drugbank_id The product of the reaction. May be a drug or a metabolite.
right_drugbank_name
parent_key drugbank id

Details

Each drug may have one or more reaction.

Source

[Drugbank Documentation](#)

Salts_Drug

Drug Salts

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.

Usage

Salts_Drug

Format

a tibble with 8 variables:

drugbank-id DrugBank identifiers 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

parent_key drugbank id

Details

Each drug may have one or more salt.

Source

[Drugbank Documentation](#)

Sequences_Drug

Drug Sequences

Description

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

Usage

Sequences_Drug

Format

a tibble with 3 variables:

sequence

format

parent_key drugbank id

Details

Each drug may have one or more sequence.

Describes peptide sequences of biotech drugs. The sequence variable contains a textual representation of the sequence, in the format described by the format variable. Currently, only the **FASTA** format is used.

Source

[Drugbank Documentation](#)

SNP_Adverse_Drug_Reactions_Drug

SNP Adverse Drug Reactions

Description

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

Usage

SNP_Adverse_Drug_Reactions_Drug

Format

a tibble with 9 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.

parent_key [drugbank id](#)

Details

Each drug may have one or more SNP Adverse.

Source

[Drugbank Documentation](#)

SNP_Effects_Drug

Drug SNP Effects

Description

A list of single nucleotide polymorphisms (SNPs) relevant 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.

Usage

SNP_Effects_Drug

Format

a tibble with 9 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 A written description of the SNP effects.

pubmed-id Reference to [PubMed](#) article

description A written description of the SNP effects

parent_key [drugbank id](#)

Details

Each drug may have one or more SNP Effect.

Source

[Drugbank Documentation](#)

Synonyms_Drug

Drugs Synonyms

Description

Other names or identifiers that are associated with the associated Drug

Usage

Synonyms_Drug

Format

a tibble with 4 variables:

synonym alternative name

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

Details

Each element may have one or more synonyms.

Source

[Drugbank Documentation](#)

Index

* datasets

- actions, [3](#)
 - Affected_Organisms_Drug, [4](#)
 - AHFS_Codes_Drug, [4](#)
 - articles, [5](#)
 - ATC_Codes_Drug, [6](#)
 - attachments, [6](#)
 - books, [7](#)
 - Calculated_Properties_Drug, [8](#)
 - Categories_Drug, [10](#)
 - cett, [10](#)
 - Classifications_Drug, [11](#)
 - Dosages_Drug, [13](#)
 - Drugs, [13](#)
 - Drugs_Pathway_Drug, [14](#)
 - Enzymes_Pathway_Drug, [15](#)
 - Enzymes_Reactions_Drug, [15](#)
 - Experimental_Properties_Drug, [16](#)
 - ext_id, [17](#)
 - External_Links_Drug, [17](#)
 - Food_Interactions_Drug, [19](#)
 - go, [20](#)
 - Groups_Drug, [21](#)
 - Interactions_Drug, [22](#)
 - International_Brands_Drug, [22](#)
 - links, [23](#)
 - Manufacturers_Drug, [24](#)
 - Mixtures_Drug, [25](#)
 - Packagers_Drug, [25](#)
 - Patents_Drug, [26](#)
 - Pathways_Drug, [27](#)
 - PDB_Entries_Drug, [27](#)
 - pfam, [28](#)
 - Pharmacology, [29](#)
 - poly_syn, [31](#)
 - polypeptide, [30](#)
 - Prices_Drug, [32](#)
 - Products_Drug, [33](#)
 - Reactions_Drug, [34](#)
 - Salts_Drug, [35](#)
 - Sequences_Drug, [36](#)
 - SNP_Adverse_Drug_Reactions_Drug, [36](#)
 - SNP_Effects_Drug, [37](#)
 - Synonyms_Drug, [38](#)
-
- actions, [3](#)
 - Actions_Carrier_Drug (actions), [3](#)
 - Actions_Enzyme_Drug (actions), [3](#)
 - Actions_Target_Drug (actions), [3](#)
 - Actions_Transporter_Drug (actions), [3](#)
 - Affected_Organisms_Drug, [4](#)
 - AHFS_Codes_Drug, [4](#)
 - articles, [5](#)
 - Articles_Carrier_Drug (articles), [5](#)
 - Articles_Drug (articles), [5](#)
 - Articles_Enzyme_Drug (articles), [5](#)
 - Articles_Target_Drug (articles), [5](#)
 - Articles_Transporter_Drug (articles), [5](#)
 - ATC_Codes_Drug, [6](#)
 - Attachments (attachments), [6](#)
 - attachments, [6](#)
 - Attachments_Carriers (attachments), [6](#)
 - Attachments_Enzymes (attachments), [6](#)
 - Attachments_Targets (attachments), [6](#)
 - Attachments_Transporters (attachments), [6](#)
-
- books, [7](#)
 - Books_Drug (books), [7](#)
-
- Calculated_Properties_Drug, [8](#)
 - Carriers_Drug (cett), [10](#)
 - Categories_Drug, [10](#)
 - cett, [10](#)
 - Classifications_Drug, [11](#)
 - covid19dbcand, [12](#)
-
- Dosages_Drug, [13](#)

- Drugs, [13](#)
- Drugs_Pathway_Drug, [14](#)
- Enzymes_Drug (cett), [10](#)
- Enzymes_Pathway_Drug, [15](#)
- Enzymes_Reactions_Drug, [15](#)
- Experimental_Properties_Drug, [16](#)
- ext_id, [17](#)
- External_Identifiers_Drug (ext_id), [17](#)
- External_Identifiers_Polypeptide_Carrier_Drug (ext_id), [17](#)
- External_Identifiers_Polypeptide_Enzyme_Drug (ext_id), [17](#)
- External_Identifiers_Polypeptide_Target_Drug (ext_id), [17](#)
- External_Identifiers_Transporter_Drug (ext_id), [17](#)
- External_Links_Drug, [17](#)
- Food_Interactions_Drug, [19](#)
- go, [20](#)
- GO_Classifiers_Polypeptide_Carrier_Drug (go), [20](#)
- GO_Classifiers_Polypeptide_Target_Drug (go), [20](#)
- GO_Classifiers_Polypeptide_Transporter_Drug (go), [20](#)
- GO_Classifiers_Polypeptides_Enzyme_Drug (go), [20](#)
- Groups_Drug, [21](#)
- Interactions_Drug, [22](#)
- International_Brands_Drug, [22](#)
- links, [23](#)
- Links_Carrier_Drug (links), [23](#)
- Links_Drug (links), [23](#)
- Links_Enzyme_Drug (links), [23](#)
- Links_Target_Drug (links), [23](#)
- Links_Transporter_Drug (links), [23](#)
- Manufacturers_Drug, [24](#)
- Mixtures_Drug, [25](#)
- Packagers_Drug, [25](#)
- Patents_Drug, [26](#)
- Pathways_Drug, [27](#)
- PDB_Entries_Drug, [27](#)
- pfam, [28](#)
- PFAMS_Polypeptid_Transporter_Drug (pfam), [28](#)
- PFAMS_Polypeptide_Carrier_Drug (pfam), [28](#)
- PFAMS_Polypeptide_Target_Drug (pfam), [28](#)
- PFAMS_Polypeptides_Enzyme_Drug (pfam), [28](#)
- Pharmacology, [29](#)
- poly_syn, [31](#)
- polypeptide, [30](#)
- Polypeptide_Target_Drug (polypeptide), [30](#)
- Polypeptides_Carrier_Drug (polypeptide), [30](#)
- Polypeptides_Enzyme_Drug (polypeptide), [30](#)
- Polypeptides_Transporter_Drug (polypeptide), [30](#)
- Prices_Drug, [32](#)
- Products_Drug, [33](#)
- Reactions_Drug, [34](#)
- Salts_Drug, [35](#)
- Sequences_Drug, [36](#)
- SNP_Adverse_Drug_Reactions_Drug, [36](#)
- SNP_Effects_Drug, [37](#)
- Synonyms_Drug, [38](#)
- Synonyms_Polypeptide_Carrier_Drug (poly_syn), [31](#)
- Synonyms_Polypeptide_Target_Drug (poly_syn), [31](#)
- Synonyms_Polypeptide_Transporter_Drug (poly_syn), [31](#)
- Synonyms_Polypeptides_Enzyme_Drug (poly_syn), [31](#)
- Targets_Drug (cett), [10](#)
- Textbooks_Carrier_Drug (books), [7](#)
- Textbooks_Enzyme_Drug (books), [7](#)
- Textbooks_Target_Drug (books), [7](#)
- Textbooks_Transporter_Drug (books), [7](#)
- Transporters_Drug (cett), [10](#)