

# Package: covid19dbcand (via r-universe)

October 10, 2024

**Type** Package

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

**Version** 0.1.1

**Depends** R (>= 3.1)

**Maintainer** Mohammed Ali <moh\_fcis@yahoo.com>

**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

**Repository** <https://epiverse-connect.r-universe.dev>

**RemoteUrl** <https://github.com/MohammedFCIS/covid19dbcand>

**RemoteRef** HEAD

**RemoteSha** 0d7ea2ee6db9b274f04a7b1a7d31447c45be0188

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---

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

**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:

<b>Property</b>	<b>Description</b>
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 <b>ALOGPS</b> .
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 system.
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 between -0.4 and 5.6, the number of hydrogen bond donors is less than 5, and the number of hydrogen bond acceptors is less than 10.
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 5, 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](#)

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

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**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>
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---

**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:

<b>Property</b>	<b>Description</b>
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 Unites 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	<i>PFAMs</i>
------	--------------

---

**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.

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 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<sub>max</sub>), and time to maximum concentration (T<sub>max</sub>).

**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.

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.

**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](#)

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