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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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

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NeedsCompilation no

Author Mohammed Ali [aut, cre]

Repository CRAN

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Drug Carriers/ Enzymes/ Targets/ Transporters related Actions

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
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 | Drug related ATC Codes

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 | Drugs/ Carriers/ Enzymes/ Targets/ Transporters Attachments

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

<table>
<thead>
<tr>
<th></th>
<th>Drugs/ Carriers/ Enzymes/ Targets/ Transporters related Books</th>
</tr>
</thead>
</table>

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:

<table>
<thead>
<tr>
<th>Property</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>logP</td>
<td>The predicted partition coefficient (LogP) based on the ratio of solubility of the molecule in 1-octanol compared to water; predicted by ALOGPS.</td>
</tr>
<tr>
<td>logS</td>
<td>The predicted solubility (LogS) of the molecule; predicted by ALOGPS.</td>
</tr>
<tr>
<td>IUPAC Name</td>
<td>The predicted International Union of Pure and Applied Chemistry (IUPAC) nomenclature for the molecule; predicted by ChemAxon.</td>
</tr>
<tr>
<td>Traditional IUPAC Name</td>
<td>The non-systematic (or common) name for the molecule, which is not recognized by any formal nomenclature system; imported from ChemAxon.</td>
</tr>
<tr>
<td>Molecular Weight</td>
<td>The predicted ratio of the average mass of one molecule of an element or compound to one twelfth of the mass of an atom of carbon-12; calculated by ChemAxon.</td>
</tr>
<tr>
<td>Monoisotopic Weight</td>
<td>The predicted mass of the most abundant isotope of the drug; calculated by ChemAxon.</td>
</tr>
<tr>
<td>SMILES</td>
<td>The simplified molecular-input line-entry system (SMILES) is a line notation used for describing chemical structures.</td>
</tr>
<tr>
<td>InChI</td>
<td>A prediction of the IUPAC International Chemical Identifier (InChI); imported by ChemAxon.</td>
</tr>
<tr>
<td>InChIKey</td>
<td>The condensed digital representation of the IUPAC International Chemical Identifier (InChI); imported from ChemAxon.</td>
</tr>
<tr>
<td>Polar Surface Area (PSA)</td>
<td>A descriptor, based on the polarized atoms of the molecule, that allows estimation of transport properties.</td>
</tr>
<tr>
<td>Refractivity</td>
<td>The predicted molar refractivity of the molecule, which is strongly related to the volume of the molecule.</td>
</tr>
<tr>
<td>Polarizability</td>
<td>The predicted relative tendency of the electron cloud (charge distribution) of the molecule to be distorted by an external electric field; polarizability values predicted by ChemAxon.</td>
</tr>
<tr>
<td>Rotatable Bond Count</td>
<td>The predicted number of rotatable bonds in the molecule; predicted by ChemAxon. Unsaturated bonds, aromatic rings, and those connecting two hindered aromatic rings (having at least three ortho substituents) are considered non-rotatable.</td>
</tr>
<tr>
<td>H Bond Acceptor Count</td>
<td>A calculation of the sum of the hydrogen bond acceptor atoms. An acceptor atom always has a lone electron pair/lone electron pairs that is capable of establishing a hydrogen bond. Predicted by ChemAxon.</td>
</tr>
<tr>
<td>H Bond Donor Count</td>
<td>A calculation of the sum of the atoms in the molecule which have hydrogen bond donor properties.</td>
</tr>
<tr>
<td>pKa (strongest acidic)</td>
<td>The strongest acidic pka value of the molecule; predicted by ChemAxon.</td>
</tr>
<tr>
<td>pKa (strongest basic)</td>
<td>The strongest basic pka value of the molecule; predicted by ChemAxon.</td>
</tr>
<tr>
<td>Physiological Charge</td>
<td>Charge of the molecule at physiological pH; predicted by ChemAxon.</td>
</tr>
<tr>
<td>Number of Rings</td>
<td>A calculation of the number of rings in the molecule; predicted by ChemAxon.</td>
</tr>
<tr>
<td>Bioavailability</td>
<td>Fraction of administered dose that is predicted to reach the systemic circulation; predicted by ChemAxon.</td>
</tr>
<tr>
<td>Rule of Five</td>
<td>A reflection of the absorption or permeation of a molecule; considered “yes” when the molecular weight is below 500; predicted by ChemAxon.</td>
</tr>
<tr>
<td>Ghose Filter</td>
<td>A filter that defines drug-likeness constraints as follows: calculated log P is between -0.4 and 5.6, molar refractivity is between 40 and 130, and the total number of atoms is between 20 and 70. Imported from ChemAxon.</td>
</tr>
<tr>
<td>MDDR-Like Rule</td>
<td>Indicates compliance of drug-like characteristics based on number of rings, rigid bonds and rotatable bonds.</td>
</tr>
</tbody>
</table>

Source

Drugbank Documentation
**Categories_Drug**

*Drug Categories General categorizations of the drug*

**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**

*Carriers/ Enzymes/ Targets/ Transporters*

**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
Classifications_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: 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.html
**Dosages_Drug**

**Description**

Each drug may have one or more dosages.

**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**

**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.
Drugs_Pathway_Drug

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

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

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
**Enzymes_Pathway_Drug**

**Source**

Drugbank Documentation

**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**

**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
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:

<table>
<thead>
<tr>
<th>kind</th>
<th>Name of the property</th>
</tr>
</thead>
<tbody>
<tr>
<td>value</td>
<td>Drug properties that have been experimentally proven</td>
</tr>
<tr>
<td>source</td>
<td>Reference to the source of this experimental data</td>
</tr>
<tr>
<td>parent_key</td>
<td>drugbank key</td>
</tr>
</tbody>
</table>

Details

The following experimental properties are provided:

<table>
<thead>
<tr>
<th>Property</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water Solubility</td>
<td>The experimentally determined aqueous solubility of the molecule</td>
</tr>
<tr>
<td>Molecular Formula</td>
<td>Protein formula of Biotech drugs</td>
</tr>
<tr>
<td>Molecular Weight</td>
<td>Protein weight of Biotech drugs</td>
</tr>
<tr>
<td>Melting Point</td>
<td>The experimentally determined temperature at which the drug molecule changes from solid to liquid at atmospheric pressures</td>
</tr>
<tr>
<td>Boiling Point</td>
<td>The experimentally determined temperature at which the drug molecule changes from liquid to gas at atmospheric pressures</td>
</tr>
<tr>
<td>Hydrophobicity</td>
<td>The ability of a molecule to repel water rather than absorb or dissolve water</td>
</tr>
<tr>
<td>Isoelectric Point</td>
<td>The pH value at which the net electric charge of a molecule is zero</td>
</tr>
<tr>
<td>caco2 Permeability</td>
<td>A continuous line of heterogeneous human epithelial colorectal adenocarcinoma cells, CAC02 cells are often used as an assay for drug absorption</td>
</tr>
<tr>
<td>pKa</td>
<td>The experimentally determined pKa value of the molecule</td>
</tr>
<tr>
<td>logP</td>
<td>The experimentally determined partition coefficient (LogP) based on the ratio of solubility of the molecule in water and 1-octanol</td>
</tr>
<tr>
<td>logS</td>
<td>The intrinsic solubility of a given compound is the concentration in equilibrium with its solid phase that the compound has in a given solvent</td>
</tr>
<tr>
<td>Radioactivity</td>
<td>The property to spontaneously emit particles (alpha, beta, neutron) or radiation (gamma, K capture), or both</td>
</tr>
</tbody>
</table>

Source

Drugbank Documentation
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

<table>
<thead>
<tr>
<th>ext_id</th>
<th>External Identifiers for Drugs/ Carriers/ Enzymes/ Targets/ Transporters</th>
</tr>
</thead>
</table>

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
Food_Interceptor_Drug

- ChemSpider
- BindingDB
- National Drug Code Directory
- GenBank
- PharmGKB
- PDB
- Guide to Pharmacology
- ZINC
- RxCUI

Source
Drugbank Documentation

Food_Interceptor_Drug

**Drug Food Interactions**

---

**Description**

Description of interactions this drug has with food.

**Usage**

Food_Interceptor_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
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.

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

---

<table>
<thead>
<tr>
<th>links</th>
<th>Drugs/ Carriers/ Enzymes/ Targets/ Transporters related Links</th>
</tr>
</thead>
</table>

**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

Drugsbank 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

Drugsbank Documentation
Mixtures_Drug

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

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

---

<table>
<thead>
<tr>
<th>Patents_Drug</th>
<th>Drug Patent</th>
</tr>
</thead>
</table>

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

**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

**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

<table>
<thead>
<tr>
<th>pfam</th>
<th>PFAMs</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
</tr>
</tbody>
</table>

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**

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
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 (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 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

<table>
<thead>
<tr>
<th>polypeptide</th>
<th>Polypeptide</th>
</tr>
</thead>
</table>

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:

<table>
<thead>
<tr>
<th>id</th>
<th>Universal Protein Resource (UniProt) identifier</th>
</tr>
</thead>
<tbody>
<tr>
<td>source</td>
<td>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.</td>
</tr>
<tr>
<td>name</td>
<td>general_function General summary of the physiological function of the polypeptide</td>
</tr>
<tr>
<td>specific_function</td>
<td>A more specific description of the polypeptide’s physiological function within the cell.</td>
</tr>
<tr>
<td>gene_name</td>
<td>The short name commonly associated with the associated gene. Eg. PTGS1.</td>
</tr>
<tr>
<td>locus</td>
<td>The specific chromosomal location or position of the gene’s sequence on a chromosome.</td>
</tr>
<tr>
<td>cellular_location</td>
<td>The cellular location of the polypeptide.</td>
</tr>
</tbody>
</table>
**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

<table>
<thead>
<tr>
<th>Prices_Drug</th>
<th>Drug Prices</th>
</tr>
</thead>
</table>

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.
- **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

<table>
<thead>
<tr>
<th>Reactions_Drug</th>
<th>Drug Reactions</th>
</tr>
</thead>
</table>

### 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
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  

### 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

### 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

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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