Package: covid19dbcand (via r-universe)

September 11, 2024

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

Repository https://interstellar-consultation-services.r-universe.dev

RemoteUrl https://github.com/interstellar-consultation-services/covid19dbcand

RemoteRef HEAD

RemoteSha 0d7ea2ee6db9b274f04a7b1a7d31447c45be0188

Contents

`actions` *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

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 *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 *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-oct
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
Traditional IUPAC Name	The non-systematic (or common) name for the molecule, which is not recognized by any formal r
Molecular Weight	The predicted ratio of the average mass of one molecule of an element or compound to one twelft
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
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); imp
Polar Surface Area (PSA)	A descriptor, based on the polarized atoms of the molecule, that allows estimation of transport pro
Refractivity	The predicted molar refractivity of the molecule, which is strongly related to the volume of the m
Polarizability	The predicted relative tendency of the electron cloud (charge distribution) of the molecule to be d
Rotatable Bond Count	The predicted number of rotatable bonds in the molecule; predicted by ChemAxon. Unsaturated b
H Bond Acceptor Count	A calculation of the sum of the hydrogen bond acceptor atoms. An acceptor atom always has a lo
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 Che
Rule of Five	A reflection of the absorption or permeation of a molecule; considered "yes" when the molecular
Ghose Filter	A filter that defines drug-likeness constraints as follows: calculated log P is between -0.4 and 5.6,
MDDR-Like Rule	Indicates compliance of drug-like characteristics based on number of rings, rigid bonds and rotata

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
```

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 *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

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 at
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/ Transporters*

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 *Drugs/ Carriers/ Enzymes/ Targets/ Transporters related Links*

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 *Drug Mixture*

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 *Drug Packagers*

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` *Drug Pathways*

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` *Drug PDB Entries*

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.

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 (Cmax), and time to maximum concentration (Tmax).

half-life The period of time it takes for the amount of drug in the body to be reduced by one half. Provides a description of how quickly the drug is being eliminated and how much is available in the bloodstream.

protein-binding A description of the drug's affinity for plama proteins and the proportion of the drug that is bound to them when in circulation within the body.

route_of_elimination A description of the pathway that is used to excrete the drug from the body. Common pharmacokinetic parameters used to evaluate excretion include elemination half life, renal clearance, and tracking of radiolabelled compounds through the renal and GI system.

volume_of_distribution The Vd of a drug represents the degree to which it is distributed into body tissue compared to the plasma.

clearance A pharmacokinetic measurement of the rate of removal of the drug from plasma, expressed as mL/min; reflects the rate of elimination of the drug.

drugbank_id drugbank id

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 *Drug Reactions*

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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