toxvaldbmain

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```
Type Package
Title Builds the ToxValDB V9.5 Database
Version 9.5
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Description
      ToxValDB is a database containing quantitative records form in vivo toxicology studies from
      many sources. The database has 2 main parts - toxval_source containing
      source data in separate tables, and the main toxval schema which combines data from multi-
      ple sources
      into a single format. This project moves data from toxval_source to toxval.
      Data is read from files or other databases into toxval_source and then pulled
      into toxval where terms are converted to standard values. The ToxValDB SOPs describe in more
     detail how to run the code. This version is setup to build ToxValDB v9.5
Imports DBI,
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Encoding UTF-8
LazyData true
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```

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Suggests knitr, rmarkdown

VignetteBuilder knitr

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Description

Check CAS RN validity via checksum method

For a suspected CAS RN, determine validity by calculating final digit checksum

Usage

```
cas\_checkSum(x, checkLEN = TRUE)
```

Arguments

chr. Input vector of values to check. Standard CAS notation using hyphens is fine, as #' all non-digit characters are stripped for checksum calculation. Each element of x should contain #' only one suspected CAS RN to check.

checkLEN logi. Should the function check that the non-digit characters of x are at least 4,

but no #' more than 10 digits long? Defaults to TRUE. #'

Details

This function performs a very specific type of check for CAS validity, namely whether the final digit checksum follows the CAS standard. By default, it also ensures that the digit length is compatible with CAS standards. It does nothing more.

This means that there is no check for valid CAS format. Use the cas_detect function to check CAS format beforehand, or write your own function if necessary.

Value

A logical vector of length x denoting whether each x is a valid CAS by the checksum method. NA input values will remain NA.

Note

This is a vectorized, reasonably high-performance version of the is.cas function found in the webchem package. The functionality encompasses only the actual checksum checking of webchem::is.cas; as mentioned in details, use cas_detect to recreate the CAS format + checksum checking in webchem::is.cas. See examples.

Short of looking up against the CAS registry, there is no way to be absolutely sure that even inputs that pass the checksum test are actually registered CAS RNs. The short digit length of CAS IDs combined with the modulo 10 single- digit checksum means that even within a set of randomly generated validly-formatted CAS entities, ~10% will pass checksum.

See Also

```
str_detect, str_pad
```

Examples

```
cas_good <- c("71-43-2", "18323-44-9", "7732-18-5") #benzene, clindamycin, water cas_bad <- c("61-43-2", "18323-40-9", "7732-18-4") #single digit change from good cas_checkSum(c(cas_good, cas_bad))
```

```
check.toxval_type.route.units
```

Output distinct combinations of toxval_type, exposure_route, and tox-val_units to check

Description

Output distinct combinations of toxval_type, exposure_route, and toxval_units to check

Usage

```
check.toxval_type.route.units(
  toxval.db,
  source = NULL,
  subsource = NULL,
  load.dict = "Repo/dictionary/toxval_type.route.units.dictionary.xlsx"
)
```

Arguments

toxval.db The version of toxvaldb to use.

source Source to check

subsource Subsource to check (NULL default)

load.dict Name of dictionary containing expected combinations, or NULL if dictionary

should not be read

chem.check.v2 7

chem.check.v2

Check the chemicals from a file Names with special characters are cleaned and trimmed CASRN are fixed (dashes put in, trimmed) and check sums are calculated The output is sent to a file called chemcheck.xlsx in the source data file One option for using this is to edit the source file until no errors are found

Description

Check the chemicals from a file Names with special characters are cleaned and trimmed CASRN are fixed (dashes put in, trimmed) and check sums are calculated The output is sent to a file called chemcheck.xlsx in the source data file One option for using this is to edit the source file until no errors are found

Usage

```
chem.check.v2(res0, in_source = NULL, verbose = FALSE)
```

Arguments

res0 The data frame in which chemicals names and CASRN will be replaced

in_source The source to be processed. If source=NULL, process all sources

verbose If TRUE, print diagnostic messages

Value

Return a list with fixed CASRN and name and flags indicating if fixes were made: res0=res0,name.OK=name.OK,casrn.OK=o

```
clean.last.character clean.last.character
```

Description

Clean unneeded characters from the end of a string

Usage

```
clean.last.character(x)
```

Arguments

x String to be cleaned

Details

DETAILS

Value

The cleaned string

See Also

```
str\_trim
```

Examples

```
## Not run:
if(interactive()){
  #EXAMPLE1
  }
## End(Not run)
```

clean.toxval.by.source

Delete a portion of the contents of the toxval database

Description

Delete a portion of the contents of the toxval database

Usage

```
clean.toxval.by.source(toxval.db, source)
```

Arguments

toxval.db The version of toxval from which the data is deleted.

source The data source name

Value

The database will be altered

compare.versions 9

compare.versions

Compare versions of toxval

Description

Compare versions of toxval

Usage

```
compare.versions(db1, db2)
```

Arguments

db1 The old version of the database
db2 The new version of the database

duplicate.hunter

Diagnose duplicates

Description

Diagnose duplicates

Usage

```
duplicate.hunter(toxval.db, source = NULL, source_table = NULL)
```

Arguments

toxval.db Database version

source The source to be updated

Value

Write a file with the results

ecotox.select.study.duration

ECOTOX Select study_duration

Description

Function to select the appropriate study_duration value from conc1_* fields

Usage

```
ecotox.select.study.duration(in_data)
```

Arguments

in_data

Input ECOTOX dataframe

Value

Processed dataframe with new study_duration_values, units, and qualitifer fields

ecotox.select.toxval.numeric

ECOTOX Select toxval_numeric

Description

Function to select the appropriate toxval_numeric value from conc1_* fields

Usage

```
ecotox.select.toxval.numeric(in_data)
```

Arguments

in_data

Input ECOTOX dataframe

Value

Processed dataframe with new toxval_numeric, units, and qualitifer fields

ecotox.species.dictionary

ecotox.species.dictionary

Extract the ECOTOX species dictionary from the ECOTOX data

Description

Extract the ECOTOX species dictionary from the ECOTOX data

Usage

```
ecotox.species.dictionary(toxval.db, do.load = F, sys.date = "2023-05-03")
```

Arguments

toxval.db	The version of toxval into which the tables are loaded.
do.load	If TRUE, load the data from the input file and put into a global variable
source.db	The version of toxval source - used to manage chemicals
verbose	Whether the loaded rows should be printed to the console.
log	If TRUE, send output to a log file

export.all.by.source Build a data frame of the data from toxval and export by source as a series of xlsx files

Description

Build a data frame of the data from toxval and export by source as a series of xlsx files

Usage

```
export.all.by.source(toxval.db, source = NULL, subsource = NULL)
```

Arguments

toxval.db	Database version
source	The source to be updated
subsource	The subsource to be updated #' @return for each source writes an Excel file with the name/export/export_by_source_data/toxval_all_toxval.db_source.xlsx

12 export.for.oppt

```
export.for.missing.species
```

Export the records with missing species and point of departure values

Description

Export the records with missing species and point of departure values

Usage

```
export.for.missing.species(toxval.db, source = NULL)
```

Arguments

toxval.db Database version

source The source to be updated #' @return for each source writes an Excel file with

the name ../export/export_by_source_data/toxval_all_toxval.db_source.xlsx

export.for.oppt

Build a data frame of the PODs and exports as xlsx

Description

Build a data frame of the PODs and exports as xlsx

Usage

```
export.for.oppt(toxval.db, file.name = "TSCA PICS")
```

Arguments

toxval.db Database version

file.name If not NA, this is a file containing chemicals, and only those chemicals will be

exported

Value

writes an Excel file with the name ../export/toxval_pod_summary_[human_eco]_Sys.Date().xlsx

export.for.toxval.qc 13

export.for.toxval.qc Build a data frame of the PODs and exports as xlsx

Description

Build a data frame of the PODs and exports as xlsx

Usage

```
export.for.toxval.qc(toxval.db, source = NULL)
```

Arguments

toxval.db Database version

human_eco Either 'human health' or 'eco'

file.name If not NA, this is a file containing chemicals, and only those chemicals will be

exported

Value

writes an Excel file with the name ../export/toxval_pod_summary_[human_eco]_Sys.Date().xlsx

```
export.for.toxvaldb.manuscript
```

Build a data frame of the data for the toxval manuscript

Description

Build a data frame of the data for the toxval manuscript

Usage

```
export.for.toxvaldb.manuscript(toxval.db)
```

Arguments

toxval.db Database version

source The source to be updated

Value

Write a file with the results

14 export.missing.strains

```
export.missing.dictionary.entries
```

Find "original" values that have not been included in the dictionaries and export them

Description

Find "original" values that have not been included in the dictionaries and export them

Usage

```
export.missing.dictionary.entries(
  toxval.db,
  source = NULL,
  subsource = NULL,
  report.only = FALSE
)
```

Arguments

toxval.db The version of toxval in which the data is altered. source The source to be fixed. If source=NULL, fix all sources

subsource The subsource to be fixed (NULL default)

report.only Whether to report or write/export data. Default is FALSE (write/export data)

Value

An excel file in dictionaries with the missing entries (if report.only=TRUE, return tibble) "missing dictionary entries Sys.Date.xlsx"

```
export.missing.strains
```

Set the strain information in toxval

Description

Set the strain information in toxval

Usage

```
export.missing.strains(toxval.db, date_string = "2024-02-27")
```

Arguments

```
toxval.db The version of the database to use date_string The date of the latest dictionary version
```

export.missing.toxval_type

Export any toxval_types that are not in the toxval_type dictionary

Description

Export any toxval_types that are not in the toxval_type dictionary

Usage

```
export.missing.toxval_type(toxval.db, report.only = FALSE)
```

Arguments

toxval.db The version of toxval in which the data is altered.

report.only Whether to report or write/export data. Default is FALSE (write/export data)

Value

An excel file in dictionaries with the missing entries (if report.only=TRUE, return tibble) "dictionary/missing/missing_toxval_type Sys.Date.xlsx"

```
export.toxvaldb.subset
```

Build a data frame of the data from toxval for a subset of chemicals

Description

Build a data frame of the data from toxval for a subset of chemicals

Usage

```
export.toxvaldb.subset(toxval.db, filename)
```

Arguments

toxval.db Database version

filename The name of the file the be imported - should be a short name that will be used

in the output filename. This is an xlsx file and needs a column labeled dtxsid

Value

Write a file with the results

Description

Pull updated field information for source info dictionary

Usage

```
export.update.source.info(toxval.db, source.db, dict_date = "2024-08-28")
```

Arguments

toxval.db Database version

source.db The source to be updated

dict_date Date stamp of the dictionary file to update

Value

Overwrite existing source info dictionary with updated fields

```
fill.chemical.by.source
```

Fill the chemical table

Description

Fill the chemical table

Usage

```
fill.chemical.by.source(toxval.db, source, verbose = TRUE)
```

Arguments

toxval.db The version of toxvaldb to use.

source The source to be used

verbose If TRUE, print out extra diagnostic messages

fill.toxval.defaults 17

Description

Set Toxval Defaults

Usage

```
fill.toxval.defaults(toxval.db, mat)
```

Arguments

toxval.db The version of toxval from which to set defaults.

mat An input matrix of data

Value

The data matrix afer fixing

```
fill.toxval.defaults.global.by.source

Set Toxval Defaults globally, replacing blanks with -
```

Description

Set Toxval Defaults globally, replacing blanks with -

Usage

```
fill.toxval.defaults.global.by.source(
  toxval.db,
  source = NULL,
  subsource = NULL
)
```

Arguments

toxval.db The version of toxval from which to set defaults.

source The source to be fixed

subsource The subsource to be fixed (NULL default)

```
fix.all.param.by.source
```

Alter the contents of toxval according to an excel dictionary file with fields - exposure_method, exposure_route, sex,strain, study_duration_class, study_duration_units, study_type, toxval_type, exposure_form, media, toxval_subtype

Description

Alter the contents of toxval according to an excel dictionary file with fields - exposure_method, exposure_route, sex,strain, study_duration_class, study_duration_units, study_type, toxval_type, exposure_form, media, toxval_subtype

Usage

```
fix.all.param.by.source(
  toxval.db,
  source = NULL,
  subsource = NULL,
  fill.toxval_fix = TRUE
)
```

Arguments

toxval.db The version of toxval in which the data is altered.

source The source to be fixed. If source=NULL, fix all sources

subsource The subsource to be fixed (NULL default)

fill.toxval_fix

If TRUE (default) read the dictionaries into the toxval fix table

Value

The database will be altered

```
fix.associated.pod.critical_effect

Appends associated POD information to critical_effect for derived
```

Description

Appends associated POD information to critical_effect for derived toxval_types

toxval_types

fix.casrn 19

Usage

```
fix.associated.pod.critical_effect(res, map_fields)
```

Arguments

res The data to be altered

fix.casrn fix.casrn

Description

Fix a CASRN that has one of several problems

Usage

```
fix.casrn(casrn, cname = "", verbose = FALSE)
```

Arguments

casrn Input CASRN to be fixed cname An optional chemical name verbose if TRUE, print the input values

Details

DETAILS

Value

the fixed CASRN

See Also

reexports

Examples

```
## Not run:
if(interactive()){
  fix.casrn("107028")
  # Expected output "107-02-8"
}
## End(Not run)
```

```
fix.critical_effect.icf.by.source
```

standardize critical_effect in toxval table based on icf dictionary and toxval critical effects dictionary

Description

standardize critical_effect in toxval table based on icf dictionary and toxval critical effects dictionary

Usage

```
fix.critical_effect.icf.by.source(toxval.db, source, subsource = NULL)
```

Arguments

toxval.db The version of toxvaldb to use.

source THe source to be fixed

subsource The subsource to be fixed (NULL default)

```
fix.dedup.hierarchy.by.source
```

Set qc_status as "fail" for lesser priority duplicates

Description

Set qc_status as "fail" for lesser priority duplicates

Usage

```
fix.dedup.hierarchy.by.source(
  toxval.db,
  source = NULL,
  subsource = NULL,
  priority_list = NULL,
  subsource_priority_list = NULL,
  criteria = c("dtxsid"),
  report.only = FALSE
)
```

Arguments

toxval.db The version of toxvaldb to use.

source Source to be fixed

subsource Subsource to be fixed (NULL default)

priority_list Named list describing source priority, with low priority index and high priority

value

subsource_priority_list

Named list of subsources to deprecate per source, source index/subsource value

criteria List of parameters used to make deduping decisions

report.only Whether to report or write/export data. Default is FALSE (write/export data)

```
fix.derived.toxval_type.by.source
```

Set select normalized toxval fields to '-' if the record is a select toxval_type

Description

Set select normalized toxval fields to '-' if the record is a select toxval_type

Usage

```
fix.derived.toxval_type.by.source(
  toxval.db,
  source = NULL,
  subsource = NULL,
  report.only = FALSE
)
```

Arguments

toxval.db The version of the database to use

source The source to be fixed

subsource The subsource to be fixed (NULL default)

report.only Whether to update database or only report the results. Default FALSE.

fix.empty.by.source Set all empty cells in toxval to '-'

Description

Set all empty cells in toxval to '-'

Usage

```
fix.empty.by.source(toxval.db, source = NULL, subsource = NULL)
```

Arguments

toxval.db The version of toxval in which the data is altered.

source The source to be fixed

subsource The subsource to be fixed (NULL default)

Value

The database will be altered

Description

Set all empty cells in record_source to '-'

Usage

```
fix.empty.record_source.by.source(toxval.db, source = NULL)
```

Arguments

toxval.db The version of toxval in which the data is altered.

source The source to be fixed

Value

The database will be altered

fix.exposure.params 23

Description

Fix the exposure fields: exposure_method, exposure_route, exposure_form based on a 3 column dictionary ~/dictionary/exposure_route_method_form.xlsx

Usage

```
fix.exposure.params(
  toxval.db,
  source = NULL,
  subsource = NULL,
  report.only = FALSE
)
```

Arguments

toxval.db The version of toxval in which the data is altered.

source The source to be fixed. If source=NULL, fix all sources

subsource The subsource to be fixed (NULL default)

report.only Whether to report or write/export data. Default is FALSE (write/export data)

fill.toxval_fix

If TRUE (default) read the dictionaries into the toxval_fix table

Value

The database will be altered (if report.only=TRUE, return missing entries)

```
fix.generation.by.source
```

Alter the contents of toxval according to an excel dictionary file with field generation

Description

Alter the contents of toxval according to an excel dictionary file with field generation

Usage

```
fix.generation.by.source(toxval.db, source, subsource = NULL)
```

fix.non_ascii.v2

Arguments

toxval.db The version of toxval in which the data is altered.

source The source to be processed

subsource The subsource to be processed (NULL default)

Value

The database will be altered

```
fix.human_eco.by.source
```

Fix the human_eco flag

Description

Fix the human_eco flag

Usage

```
fix.human_eco.by.source(toxval.db, source = NULL, subsource = NULL)
```

Arguments

toxval.db The version of toxval in which the data is altered.

source The source to be fixed. If NULL, fix all sources

subsource The subsource to be fixed (NULL default)

Value

The database will be altered

```
fix.non_ascii.v2 fix.non_ascii.v2
```

Description

Flag and fix non-ascii characters in the database

Usage

```
fix.non_ascii.v2(df, source)
```

Arguments

df The dataframe to be processed

source Current ToxVal source
The source to be fixed

Details

DETAILS

Value

The dataframe with non ascii characters replaced with cleaned versions

See Also

```
read.xlsx, write.xlsx str_trim stri_escape_unicode
```

Examples

```
## Not run:
if(interactive()){
  #EXAMPLE1
  }
## End(Not run)
```

```
fix.priority_id.by.source
```

Fix the priority_id in the toxval table based on source

Description

Fix the priority_id in the toxval table based on source

Usage

```
fix.priority_id.by.source(toxval.db, source = NULL, subsource = NULL)
```

Arguments

toxval.db The version of toxvaldb to use.

source The source to be fixed, If NULL, set for all sources

subsource The subsource to be fixed (NULL default)

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```
fix.qc_status.by.source
```

Fix the qa_status flag

Description

Fix the qa_status flag

Usage

```
fix.qc_status.by.source(
  toxval.db,
  source.db,
  source = NULL,
  subsource = NULL,
  reset = FALSE
)
```

Arguments

toxval.db The version of toxval in which the data is altered.

source The source to be fixed

subsource The subsource to be fixed (NULL default)

reset If TRUE, reset all values to 'pass' before setting

sourcedb The source database name

Value

The database will be altered

```
fix.replace.unicode
fix.replace.unicode
```

Description

A function to check all character fields and handle unicode symbols, either by removing them or replacing them with alphabetic equivalents.

Usage

```
fix.replace.unicode(df)
```

Arguments

df

Character vector to check/replace unicode symbols.

Details

DETAILS

Value

Returns a modified version of the input vector with unicode replacements.

See Also

```
[stri_escape_unicode][stringi::stri_escape_unicode] [str_extract][stringr::str_extract]
```

Examples

```
## Not run:
if(interactive()){
  #EXAMPLE1
  }
## End(Not run)
```

```
fix.risk_assessment_class.by.source
```

Set the risk assessment class of toxval according to an excel dictionary. Values may be set multiple times, so the excel sheet should be ordered so that the last ones to be set are last

Description

Set the risk assessment class of toxval according to an excel dictionary. Values may be et multiple times, so the excel sheet should be ordered so that the last ones to be set are last

Usage

```
fix.risk_assessment_class.by.source(
  toxval.db,
  source = NULL,
  subsource = NULL,
  restart = TRUE,
  report.only = FALSE
)
```

Arguments

toxval.db The version of toxval in which the data is altered.

source The source to be updated

subsource The subsource to be updated (NULL default)
restart If TRUE, delete all values and start from scratch

report.only Whether to report or write/export data. Default is FALSE (write/export data)

```
fix.single.param.by.source
```

Alter the contents of toxval according to an excel dictionary

Description

Alter the contents of toxval according to an excel dictionary

Usage

```
fix.single.param.by.source(
  toxval.db,
  param,
  source,
  subsource = NULL,
  ignore = FALSE,
  report.only = FALSE,
  units.data = NULL
)
```

Arguments

toxval.db The version of toxval in which the data is altered.

param The parameter value to be fixed

source The source to be fixed

subsource The subsource to be fixed (NULL default) ignore If TRUE allow missing values to be ignored

report.only Whether to report or write/export data. Default is FALSE (write/export data)
units.data A dataframe containing current units data if units are to be reported (NULL)

default)

Value

The database will be altered

```
fix.species.common_name
```

Fix issues with species common names

Description

Fix issues with species common names

fix.species.duplicates 29

Usage

```
fix.species.common_name(toxval.db)
```

Arguments

toxval.db The version of toxval into which the tables are loaded.

```
fix.species.duplicates
```

Check for species duplicates - same common name but multiple species_ids

Description

Check for species duplicates - same common name but multiple species_ids

Usage

```
fix.species.duplicates(toxval.db, source = NULL, subsource = NULL)
```

Arguments

toxval.db The version of the database to use

source The source to be checked. If source=NULL, check all sources

subsource The subsource to be checked (NULL default)

fix.species.v2

Set the species_id column in toxval

Description

This function replaces fix.species This function precedes toxvaldb.load.species

Usage

```
fix.species.v2(
  toxval.db,
  source = NULL,
  subsource = NULL,
  date_string = "2023-05-18"
)
```

Arguments

toxval.db The version of the database to use

source The source to be fixed

subsource The subsource to be fixed (NULL default)

date_string The date version of the dictionary

fix.strain.v2

Set the strain information in toxval

Description

Set the strain information in toxval

Usage

```
fix.strain.v2(
  toxval.db,
  source = NULL,
  subsource = NULL,
  date_string = "2024-04-08",
  reset = FALSE
)
```

Arguments

toxval.db The version of the database to use

source The source to be fixed. If NULL, fix for all sources

subsource The subsource to be fixed (NULL default)
date_string The date of the latest dictionary version

```
fix.study_duration.params
```

Fix the study duration fields: study_duration_value, study_duration_units, study_duration_class based on a 3 column dictionary ~/dictionary/exposure_route_method_form.xlsx

Description

Fix the study duration fields: study_duration_value, study_duration_units, study_duration_class based on a 3 column dictionary ~/dictionary/exposure_route_method_form.xlsx

fix.study_group 31

Usage

```
fix.study_duration.params(
  toxval.db,
  source = NULL,
  subsource = NULL,
  report.only = FALSE
)
```

Arguments

toxval.db The version of toxval in which the data is altered.

source The source to be fixed. If source=NULL, fix all sources

subsource The subsource to be fixed (NULL default)

report.only Whether to report or write/export data. Default is FALSE (write/export data)

fill.toxval_fix

If TRUE (default) read the dictionaries into the toxval_fix table

Value

The database will be altered

fix.study_group Set the study_group field

Description

Set the study_group field

Usage

```
fix.study_group(
  toxval.db,
  source = NULL,
  subsource = NULL,
  report.only = FALSE
)
```

Arguments

toxval.db Database version

source The source to be updated

subsource The subsource to be updated (NULL default)

report.only Whether to apply study_group fix or just report what fixes would be applied.

Value

for each source writes an Excel file with the name ../export/export_by_source_data/toxval_all_toxval.db_source.xlsx

```
fix.study_type.by.source
```

Fix the study_type using manual curation on a source-by-source basis

Description

This function replaces the original export.for_study_type and fix.study_type.manual, with the intention of making it easier to fix the study types on a source-by-source basis All of the work will happen in the directory ~/Repo/dictionary/study_type_by_source. Each source will have its own file and will not have a date attached to make maintenance easier. To start the process, run this with mode="export". This will write a source-specific file to the export_temp directory. Open either the xlsx or csv (if the xslx is corrupted) and place this file into the main directory (study_type_by_source) and edit it there as documented in the main documentation. Next run this function with mode="import". This will load your changes into the database. It is suggested that before working on a new source that the old version in the study_type_by_source get pushed to the old_versions directory

Usage

```
fix.study_type.by.source(
   toxval.db,
   mode = "export",
   source = NULL,
   subsource = NULL,
   custom.query.filter = NULL,
   report.only = FALSE
)
```

Arguments

toxval.db The version of toxval in which the data is altered.

mode Either export or import

source The source you want to work on. If NULL, this will run all sources

subsource The subsource to be fixed

custom.query.filter

Additional filters for the query. Example: custom.query.filter = paste0(" and b.human_eco='human health' and ", "e.toxval_type_supercategory in ('Point of

Departure','Lethality Effect Level','Toxicity Value')")

report.only Whether to report or write/export data. Default is FALSE (write/export data)

Value

The database will be altered

fix.trim_spaces 33

fix.trim_spaces

Trim leading and trailing blanks from all character columns

Description

Trim leading and trailing blanks from all character columns

Usage

```
fix.trim_spaces(res)
```

Arguments

toxval.db The version of toxval in which the data is altered.

source The source to be fixed. If source=NULL, fix all sources fill.toxval_fix

If TRUE (default) read the dictionaries into the toxval_fix table

Value

The database will be altered

fix.units.by.source

Do all of the fixes to units

Description

- 1. All of these steps operate on the toxval_units column.
- 2. Replace variant unit names with standard ones, running fix.single.param.new.by.source.R This fixes issues like variant names for mg/kg-day and uses the dictionary file dictionary/toxval_units_5.xlsx
- 3. Fix special characters in toxval_units
- 4. Fix issues with units containing extra characters for some ECOTOX records
- 5. Convert units that are multiples of standard ones (e.g. ppb to ppm). This uses the dictionary file dictionary/toxval_units conversions 2018-09-12.xlsx
- 6. Run conversions from molar to mg units, using MW. This uses the dictionary file dictionary/MW conversions.xlsx
- 7. Convert ppm to mg/m3 for inhalation studies. This uses the conversion Concentration (mg/m3) = 0.0409 x concentration (ppm) x molecular weight. See https://cfpub.epa.gov/ncer_abstracts/index.cfm/fuseaction/disp_This function requires htat the DSSTox external chemical_id be set
- 8. Convert ppm to mg/kg-day in toxval according to a species-specific conversion factor for oral exposures. This uses the dictionary file dictionary/ppm to mgkgday by animal.xlsx See: www10.plala.or,jp/biostatistics/1-3.doc This probbaly assumes feed rather than water
- 9. Make sure that eco studies are in mg/L and human health in mg/m3

34 generate.originals

Usage

```
fix.units.by.source(
  toxval.db,
  source = NULL,
  subsource = NULL,
  do.convert.units = FALSE,
  report.only = FALSE,
  report.extra = FALSE
)
```

Arguments

toxval.db The version of toxvaldb to use.

source Source to be fixed

subsource Subsource to be fixed (NULL default)

do.convert.units

If TRUE, so unit conversions, as opposed to just cleaning

report.only Whether to report or write/export data. Default is FALSE (write/export data)

report.extra If reporting, then choose whether to record extra conversion information (e.g.

toxval_type, mw, species_id, etc.)

Description

Duplicate any columns with '_original' Set Toxval Defaults

Usage

```
generate.originals(toxval.db, mat)
```

Arguments

toxval.db The version of toxval from which to set defaults.

mat THe matrix of data to be altered

Value

The altered input matrix

getDBConn 35

getDBConn

getDBConn

Description

Get the names the database server, user, and pass or returns error message

Usage

```
getDBConn()
```

Details

DETAILS

Value

print the database connection information

Examples

```
## Not run:
if(interactive()){
  #EXAMPLE1
  }
## End(Not run)
```

import.dictionary

import the toxval and toxval_type dictionaries

Description

import the toxval and toxval_type dictionaries

Usage

```
import.dictionary(toxval.db)
```

Arguments

toxval.db

The name of the database

36 load.dsstox

```
import.source.info.by.source
```

Load Source Info for each source into toxval The information is in the file ~/dictionary/source_info 2023-11-30.xlsx

Description

Load Source Info for each source into toxval The information is in the file \sim /dictionary/source_info 2023-11-30.xlsx

Usage

```
import.source.info.by.source(
  toxval.db,
  source = NULL,
  dict_date = "2024-08-28"
)
```

Arguments

toxval.db The version of toxval into which the source info is loaded.

source The specific source to be loaded, If NULL, load for all sources

dict_date Date stamp of the dictionary file to update

load.dsstox

Load DSSTox if needed from a file into a global variables (DSSTOX)

Description

Load DSSTox if needed from a file into a global variables (DSSTOX)

Usage

```
load.dsstox(reprocess = FALSE)
```

log_message 37

log_message

Function to combine output log with output message

Description

Function to combine output log with output message Function to combine output log with output message

Usage

```
log_message(log_df, message_df_col)
log_message(log_df, message_df_col)
```

Arguments

printCurrentFunction printCurrentFunction

Description

Print the name of the current function

Usage

```
printCurrentFunction(comment.string = NA)
```

Arguments

comment.string An optional string to be printed

Details

DETAILS

Value

None

See Also

flush.console

38 pull_jira_info

Examples

```
## Not run:
if(interactive()){
  #EXAMPLE1
  }
## End(Not run)
```

pull_jira_info

pull_jira_info

Description

Script to process CSV export of Jira into a status log

Usage

```
pull_jira_info(
    jira_project = "TOXVAL",
    in_file = NULL,
    auth_token = NULL,
    ticket_filter_list = NULL)
```

Arguments

Details

DETAILS

Value

Summary DataFrame of Jira tickets by Epic, Label, and Status

See Also

[download.file][utils::download.file], [unzip][utils::unzip] [read_csv][readr::read_csv], [cols][readr::cols] [select][dplyr::select], [contains][dplyr::contains], [mutate][dplyr::mutate], [everything][dplyr::everything], [filter][dplyr::filter], [distinct][dplyr::distinct], [left_join][dplyr::left_join], [group_by][dplyr::group_by], [summarise][dplyr::summarise], [n][dplyr::n] [unite][tidyr::unite] [str_squish][stringr::str_squish]

Examples

```
## Not run:
if(interactive()){
  out = pull_jira_info(jira_project="project_name")
}
## End(Not run)
```

```
\label{eq:qa_toxval_url_validation} qa\_toxval\_url\_validation
```

Description

Function to pull URLs and log their HTTP statuses

Usage

```
qa_toxval_url_validation(
  tbl_list = c("toxval", "record_source", "source_info"),
  db,
  log_suffix
)
```

Arguments

tbl_list List of ToxVal tables to pull URLs from, Default: c("toxval", "record_source",
"source_info")

db ToxVal database name to pull URLs from

log_suffix Suffix to add to end of log file to uniquely identify file, Default: Date stamp
from Sys.Date()

Details

DETAILS

Value

None. Log file is generated

See Also

read_excel filter, mutate, reexports, bind pivot_longer keep GET, status_code write_xlsx

40 runInsert

Examples

```
## Not run:
if(interactive()){
  qa_toxval_url_validation(tbl_list = c("toxval", "record_source", "source_info"), db="res_toxval_v94", log_suffix
}
## End(Not run)
```

runInsert

runInsert

Description

Insert a record into a database. if auto.increment=TRUE, return the auto incremented primary key of the record. otherwise, return -1

Usage

```
runInsert(query, db, do.halt = F, verbose = F, auto.increment.id = F)
```

Arguments

query a properly formatted SQL query as a string

db the name of the database

do.halt if TRUE, halt on errors or warnings verbose if TRUE, print diagnostic information

auto.increment.id

PARAM_DESCRIPTION, Default: F

auto.increment if TRUE, add the auto increment primary key even if not part of the query

Details

DETAILS

Value

Returns the database table auto incremented primary key ID

See Also

```
character(0), MySQLDriver-class
```

runInsertTable 41

Examples

```
## Not run:
if(interactive()){
  #EXAMPLE1
  }
## End(Not run)
```

runInsertTable

runInsertTable

Description

Inserts multiple rows into a database table

Usage

```
runInsertTable(mat, table, db, do.halt = TRUE, verbose = FALSE, get.id = TRUE)
```

Arguments

```
mat data frame containing the data, with the column names corresponding table name of the database table to which data will be inserted db the name of the database do.halt if TRUE, halt on errors or warnings verbose if TRUE, print diagnostic information get.id Whether to return ID or not, Default: T
```

Details

DETAILS

Value

ID or None

See Also

```
character(0), MySQLDriver-class
```

```
## Not run:
if(interactive()){
  #EXAMPLE1
  }
## End(Not run)
```

runQuery

runQuery runQuery

Description

Runs a database query and returns a result set

Usage

```
runQuery(query = NULL, db, do.halt = TRUE, verbose = FALSE)
```

Arguments

query a properly formatted SQL query as a string

db the name of the database

do.halt if TRUE, halt on errors or warnings verbose if TRUE, print diagnostic information

Details

DETAILS

Value

Query results

See Also

```
character(0), MySQLDriver-class flush.console
```

```
## Not run:
if(interactive()){
  #EXAMPLE1
  }
## End(Not run)
```

runStatement 43

runStatement	runStatement	
--------------	--------------	--

Description

Run a SQL statement, such as an ALTER or UPDATE

Usage

```
runStatement(query, db, do.halt = FALSE, verbose = FALSE)
```

Arguments

query a properly formatted SQL query as a string

db the name of the database

do.halt if TRUE, halt on errors or warnings
verbose if TRUE, print diagnostic information

Details

DETAILS

Value

None. SQL statement is run.

See Also

```
character(0), MySQLDriver-class
```

```
## Not run:
if(interactive()){
  #EXAMPLE1
  }
## End(Not run)
```

runUpdate runUpdate

runUpdate runUpdate

Description

Runs a database query and returns a result set

Usage

```
runUpdate(
  table,
  updateQuery = NULL,
  updated_df = NULL,
  db,
  do.halt = TRUE,
  verbose = FALSE,
  trigger_check = TRUE
)
```

Arguments

table table to update

updateQuery a properly formatted SQL query as a string in the form of an UPDATE INNER

JOIN

updated_df a dataframe of updated data to temporarily write to database for INNER JOIN

db the name of the database

do.halt if TRUE, halt on errors or warnings verbose if TRUE, print diagnostic information

trigger_check if FALSE, audit triggers are ignored/bypassed

Details

DETAILS

Value

None

See Also

character(0), MySQLDriver-class dbSendStatement

Examples

```
## Not run:
if(interactive()){
  #EXAMPLE1
  }
## End(Not run)
```

```
set.critical_effect_category
```

Sets the final category for each term/study_type pair in the critical_effect_terms table

Description

Sets the final category for each term/study_type pair in the critical_effect_terms table

Usage

```
set.critical_effect_category(toxval.db)
```

Arguments

toxval.db The version of toxval into which the tables are loaded.

Value

None. SQL update statement is performed

```
set.experimental_record.by.source
```

Sets experimental_record flag by source for records in toxval

Description

Sets experimental_record flag by source for records in toxval

Usage

```
set.experimental_record.by.source(toxval.db, source = NULL)
```

Arguments

toxval.db The version of toxval into which the tables are loaded.

source Name of source to set. Default NULL means set experimental record for all

sources

Value

None. SQL update statement is performed

Description

Set toxval qc_status to source table qc_status

Usage

```
set.initial.qc_status(toxval.db, source.db, source, subsource = NULL)
```

Arguments

```
toxval.db The database version to use source.db The source database name
```

source The source name

subsource The subsource to update, if desired (Default: NULL)

```
set.qc.category.by.source
```

Function for assigning QC Categories to sources in toxval via the qc_category field

Description

Function for assigning QC Categories to sources in toxval via the qc_category field

```
set.qc.category.by.source(
  toxval.db,
  source.db,
  source = NULL,
  confluence_url = "https://confluence.epa.gov/x/VuCkFg",
  confluence_access_token,
  jira_access_token
)
```

Arguments

```
toxval.db The version of toxval into which the tables are loaded.

source.db The source database to use.

source The source to set a qc_category for

confluence_url URL to QC tracking Confluence page

confluence_access_token

A personal access token for authentication in Confluence

jira_access_token

A personal access token for authentication in Jira
```

Description

Normalize study_type within study_group

Usage

```
set.study_type.by.study_group(
  toxval.db,
  source = NULL,
  subsource = NULL,
  report.only = TRUE,
  filter.matching = FALSE
)
```

Arguments

toxval.db The version of toxvaldb to use.

source Source to check

subsource Subsource to check (NULL default)

report.only Whether to alter Tox Val (FALSE) or simply record suggestions (TRUE), default

TRUE

filter.matching

Whether to ignore entries whose current study_type matches suggestion, default FALSE

```
set.supersource.export.names
```

Populate export_source_name and supersource fields in ToxVal

Description

Populate export_source_name and supersource fields in ToxVal

Usage

```
set.supersource.export.names(
  toxval.db,
  source = NULL,
  version_date = "2024-08-28"
)
```

Arguments

toxval.db The version of toxval from which to set defaults.

source The source to be fixed (if NULL then edit all sources)
version_date The date of the source_info dictionary to be used

```
set_extraction_doc_clowder_id
```

Inserts clowder document information into record_source table

Description

Inserts clowder document information into record_source table

Usage

```
set_extraction_doc_clowder_id(toxval.db, source.db, source = NULL)
```

Arguments

toxval.db The version of toxval into which the tables are loaded.

source.db The source database to use.

source Name of source to set. Default NULL means set Clowder ID for all sources

Value

None. SQL insert statement is performed

```
\verb|set_toxval_relationship_by_toxval_type| \\
```

Generic function for setting record relationships based on standardized rules

Description

Generic function for setting record relationships based on standardized rules

Usage

```
set_toxval_relationship_by_toxval_type(res, toxval.db)
```

Arguments

res The data that has relationships to be represented

toxval.db The version of toxval into which the tables are loaded.

```
source_chemical.chemidplus
```

special process to deal with source chemicals for ChemIDPlus

Description

special process to deal with source chemicals for ChemIDPlus

```
source_chemical.chemidplus(
  toxval.db,
  source.db,
  res,
  source,
  chem.check.halt = FALSE,
  casrn.col = "casrn",
  name.col = "name",
  verbose = F
)
```

Arguments

toxval.db The version of toxval into which the source info is loaded. source.db The source database version

Source. do The source database version

source The xource to be processed (ECOTOX)

chem.check.halt

If TRUE, halt if there are errors in the chemical checking

casrn.col Name of the column containing the CASRN
name.col Name of the column containing chemical names
verbose If TRUE, output extra diagnostics information

source_chemical.ecotox

special process to deal with source chemicals for ECOTOX

Description

special process to deal with source chemicals for ECOTOX

Usage

```
source_chemical.ecotox(
  toxval.db,
  source.db,
  res,
  source,
  chem.check.halt = FALSE,
  casrn.col = "casrn",
  name.col = "name",
  verbose = F
)
```

Arguments

toxval.db The version of toxval into which the source info is loaded.

source.db The source database version

source The xource to be processed (ECOTOX)

chem.check.halt

If TRUE, halt if there are errors in the chemical checking

casrn.col Name of the column containing the CASRN

name.col Name of the column containing chemical names

verbose If TRUE, output extra diagnostics information

source_chemical.extra 51

source_chemical.extra special process to deal with source chemicals for extra source (cancer, genetox, skin_eye, etc)

Description

special process to deal with source chemicals for extra source (cancer, genetox, skin_eye, etc)

Usage

```
source_chemical.extra(
  toxval.db,
  source.db,
  res,
  source,
  chem.check.halt = FALSE,
  casrn.col = "casrn",
  name.col = "name",
  verbose = FALSE
)
```

Arguments

toxval.db	The version of toxval into which the source info is loaded.
source.db	The source database version
source	The source to be processed #' @param chem.check.halt If TRUE, halt if there are errors in the chemical checking
casrn.col	Name of the column containing the CASRN
name.col	Name of the column containing chemical names
verbose	If TRUE, output extra diagnostics information

```
source_chemical.toxrefdb
```

Special process to deal with source chemicals for ToxRefDB. This will put the chemicals into the source database source_chemical table

Description

Special process to deal with source chemicals for ToxRefDB. This will put the chemicals into the source database source_chemical table

Usage

```
source_chemical.toxrefdb(
  toxval.db,
  source.db,
  res,
  source = "ToxRefDB",
  chem.check.halt = FALSE,
  casrn.col = "casrn",
  name.col = "name",
  verbose = FALSE
)
```

Arguments

toxval.db The version of toxval into which the source info is loaded.

source.db The source database version

res The dataframe to which the chemical_id sill be added

source The name of the source

chem.check.halt

If TRUE, stop if there are problems with the chemical mapping

casrn.col The name of the column containing the CASRN

name.col The name of hte column containing hte chemical name

verbose If TRUE, write out diagnostic messages

Value

Returns the input dataframe with the chemical_id added

Description

Generate the hash key for a source table based on hashing columns

Usage

```
source_hash_vectorized(res, hashing_cols)
```

Arguments

res The data frame to be processed

hashing_cols Optional list of columns to use for generating source_hash

species.qc 53

Details

DETAILS

Value

Input dataframe with new source_hash field

See Also

```
digest distinct
```

Examples

```
## Not run:
if(interactive()){
  #EXAMPLE1
  }
## End(Not run)
```

species.qc

Run some checks on the species information

Description

Run some checks on the species information

Usage

```
species.qc(toxval.db)
```

Arguments

toxval.db

The version of toxval into which the tables are loaded.

species.strain.mismap Find species and strain mismaps

Description

Find species and strain mismaps

```
species.strain.mismap(toxval.db)
```

54 toxval.config

Arguments

```
toxval.db Database version
```

Value

Write a file with the results

toxval.config

toxval.config

Description

Define a set of global variables. These include the source path (datapath) and the source databases (e.g. dev_toxval_version and dev_toxval_source_version).

Usage

```
toxval.config()
```

Details

DETAILS

Value

Returns a set of parameters to be used throughout the package

```
## Not run:
if(interactive()){
  #EXAMPLE1
  }
## End(Not run)
```

toxval.init.db 55

tables	toxval.init.db	Initialize the database. THis sill load the species, info and dictionary tables
--------	----------------	---

Description

Initialize the database. THis sill load the species, info and dictionary tables

Usage

```
toxval.init.db(toxval.db, version_info, reset = F, date_string = "2022-05-25")
```

Arguments

toxval.db The version of toxval into which the tables are loaded.

version_info Info string describing the version.

reset If TRUE, delete all content from the database

date_string The date of the dictionary versions

toxval.load.alaska_dec

Load the alaska_dec (old ACToR - flex)data from toxval sourcedb to toxval

Description

Load the alaska_dec (old ACToR - flex)data from toxval sourcedb to toxval

Usage

```
toxval.load.alaska_dec(toxval.db, source.db, log = F)
```

Arguments

toxval.db The database version to use

source.db The source database

log If TRUE, output log inoformation to a file

56 toxval.load.all

toxval.load.all

Load and process all information into ToxValDB. The entire process can be run with one command: toxval.load.all(toxval.db=...,source.db=..., do.all=TRUE) It can also be run in stages, but needs to be run in the order of the do.X parameters listed here. If any earlier step is run, all of the subsequent steps need to be rerun.

Description

Load and process all information into ToxValDB. The entire process can be run with one command: toxval.load.all(toxval.db=...,source.db=..., do.all=TRUE) It can also be run in stages, but needs to be run in the order of the do.X parameters listed here. If any earlier step is run, all of the subsequent steps need to be rerun.

Usage

```
toxval.load.all(
  toxval.db,
  source.db,
  confluence_access_token,
  jira_access_token,
  log = FALSE,
  do.init = FALSE,
  do.reset = FALSE,
  do.post = FALSE,
  do.extra = FALSE
)
```

Arguments

toxval.db	The version of toxval into which the tables are loaded.		
source.db	The version of toxval_source database from which information is pulled.		
confluence_access_token			
	A personal access token for authentication in Confluence		
jira_access_token			
	A personal access token for authentication in Jira		
log	If TRUE write the output from each load script to a log file		
do.init	If True, clean out all of the database tables		
do.reset	If TRUE, empty the database to restart		
do.load	If TRUE, load all of the source		
do.post	If TRUE, do th post-processingwork of fixing study type and risk_assessment_class		
do.extra	If TRUE, load the non-toxval data (genetox, bcfbaf, skin/eye)		

Value

Nothing is returned

```
toxval.load.atsdr.pfas.2021
```

Load data ATSDR PFAS 2021 data from toxval_source to toxval

Description

Load data ATSDR PFAS 2021 data from toxval_source to toxval

Usage

```
toxval.load.atsdr.pfas.2021(
  toxval.db,
  source.db,
  log = FALSE,
  remove_null_dtxsid = TRUE
)
```

Arguments

```
toxval.load.atsdr_mrls
```

Load the ATSDR MRLs data from toxval_source to toxval

Description

Load the ATSDR MRLs data from toxval_source to toxval

```
toxval.load.atsdr_mrls(
  toxval.db,
  source.db,
  log = FALSE,
  remove_null_dtxsid = TRUE
)
```

58 toxval.load.cancer

Arguments

toxval.db The version of toxval into which the tables are loaded.

source.db The source database to use.

log If TRUE, send output to a log file

remove_null_dtxsid

If TRUE, delete source records without curated DTXSID value

toxval.load.caloehha Load new_caloehha from toxval_source to toxval

Description

Load new_caloehha from toxval_source to toxval

Usage

```
toxval.load.caloehha(
  toxval.db,
  source.db,
  log = FALSE,
  remove_null_dtxsid = TRUE
)
```

Arguments

toxval.db The version of toxval into which the tables are loaded.

source.db The source database to use.

log If TRUE, send output to a log file

remove_null_dtxsid

If TRUE, delete source records without curated DTXSID value

toxval.load.cancer

prepare the cancer call data. The data comes form a series of files ../NIOSH/NIOSH_CARC_2018.xlsx ../IRIS/iris_cancer_call_2018-10-03.xlsx ../PPRTV_ORNL/PPRTV_ORNL cancer calls 2018-10-25.xlsx ../cancer_summary/cancer/NTP/NTP cancer clean.xlsx ../cancer_summary/cancer/IARC/IARC cancer 2018-10-29.xlsx ../cancer_summary/cancer/HealthCanada/HealthCanada_TRVs_2010_AppendixAv2.xlsx ../cancer_summary/cancer/EPA_OPP_CARC/EPA_CARC.xlsx ../cancer_summary/cancer/CalEPA/calepa_p65_cancer_only.xlsx

Description

extract all of the chemicals with cancer slope factor or unit risk with appropriate units

toxval.load.chemidplus 59

Usage

```
toxval.load.cancer(toxval.db, source.db)
```

Arguments

toxval.db The version of the database to use

toxval.load.chemidplus

Load ChemID Plus Acute data to toxval

Description

Load ChemID Plus Acute data to toxval

Usage

```
toxval.load.chemidplus(
  toxval.db,
  source.db,
  log = FALSE,
  remove_null_dtxsid = TRUE,
  do.init = FALSE
)
```

Arguments

toxval.db The database version to use

source.db The source database

log If TRUE, send output to a log file

remove_null_dtxsid

If TRUE, delete source records without curated DTXSID value

do.init if TRUE, read the data in from the file and set up the matrix

60 toxval.load.dedup

toxval.load.copper

Load Copper Manufacturers data to toxval from toxval_source

Description

Load Copper Manufacturers data to toxval from toxval_source

Usage

```
toxval.load.copper(
  toxval.db,
  source.db,
  log = FALSE,
  remove_null_dtxsid = TRUE
)
```

Arguments

toxval.db The database version to use source.db The source database log If TRUE, send output to a log file remove_null_dtxsid

If TRUE, delete source records without curated DTXSID value

toxval.load.dedup

toxval.load.dedup

Description

Perform deduping on data before it is loaded to toxval

Usage

```
toxval.load.dedup(
  res,
  dedup_fields = NULL,
  hashing_cols = toxval.config()$hashing_cols,
  delim = " |::| "
```

Arguments

res dataframe containing the source data to dedup

dedup_fields vector containing field names to dedup, Default: NULL (all fields but hashing cols)

hashing_cols vector containing field names of hashing columns, Default: toxval.config()\$hashing_cols

delim string used to separate collapsed values, Default: '!::|'

toxval.load.dod 61

Details

DETAILS

Value

dataframe containing deduped source data

See Also

```
select, group_by, summarise, context, filter, mutate, across, reexports, na_if, distinct
```

Examples

```
## Not run:
if(interactive()){
  #EXAMPLE1
  }
## End(Not run)
```

 ${\tt toxval.load.dod}$

Load the DOD data from toxval_source to toxval

Description

Load the DOD data from toxval_source to toxval

Usage

```
toxval.load.dod(toxval.db, source.db, log = FALSE, remove_null_dtxsid = TRUE)
```

Arguments

toxval.db The version of toxval into which the tables are loaded.

source.db The source database to use.

log If TRUE, send output to a log file

62 toxval.load.doe.pac

```
toxval.load.doe.benchmarks
```

Load DOE Wildlife Benchmarks data from toxval_source to toxval

Description

Load DOE Wildlife Benchmarks data from toxval_source to toxval

Usage

```
toxval.load.doe.benchmarks(
  toxval.db,
  source.db,
  log = FALSE,
  remove_null_dtxsid = TRUE
)
```

Arguments

 ${\it toxval.load.doe.pac} \quad {\it Load\ DOE\ Protective\ Action\ Criteria\ data\ from\ toxval_source\ to\ toxval}$

Description

Load DOE Protective Action Criteria data from toxval_source to toxval

```
toxval.load.doe.pac(
  toxval.db,
  source.db,
  log = FALSE,
  remove_null_dtxsid = TRUE
)
```

toxval.load.echa_iuclid

Arguments

toxval.db The version of toxval into which the tables are loaded.

source.db The source database to use.

log If TRUE, send output to a log file

remove_null_dtxsid

If TRUE, delete source records without curated DTXSID value

toxval.load.echa_iuclid

Loading the ECHA IUCLID data to toxval from toxval_source This method is different from most because there are multiple tables (one per study type) for this source

63

Description

Loading the ECHA IUCLID data to toxval from toxval_source This method is different from most because there are multiple tables (one per study type) for this source

Usage

```
toxval.load.echa_iuclid(
  toxval.db,
  source.db,
  log = FALSE,
  remove_null_dtxsid = TRUE
)
```

Arguments

toxval.db The database version to use

source.db The source database

log If TRUE, send output to a log file

remove_null_dtxsid

If TRUE, delete source records without curated DTXSID value

64 toxval.load.efsa

toxval.load.ecotox

Load ECOTOX from the datahub to toxval

Description

Load ECOTOX from the datahub to toxval

Usage

```
toxval.load.ecotox(
  toxval.db,
  source.db,
  log = FALSE,
  remove_null_dtxsid = TRUE,
  sys.date = "2024-05-30"
)
```

Arguments

toxval.db The database version to use

source.db The source database

log If TRUE, send output to a log file

remove_null_dtxsid

If TRUE, delete source records without curated DTXSID value

sys.date The version of the data to be used

toxval.load.efsa

Load EFSA data from toxval_source to toxval

Description

Load EFSA data from toxval_source to toxval

Usage

```
toxval.load.efsa(toxval.db, source.db, log = FALSE, remove_null_dtxsid = TRUE)
```

Arguments

toxval.db The version of toxval into which the tables are loaded.

source.db The source database to use.

log If TRUE, send output to a log file

toxval.load.epa_aegl 65

```
toxval.load.epa_aegl Load the EPA AEGL data from toxval_source to toxval
```

Description

Load the EPA AEGL data from toxval_source to toxval

Usage

```
toxval.load.epa_aegl(
  toxval.db,
  source.db,
  log = FALSE,
  remove_null_dtxsid = TRUE
)
```

Arguments

Description

Load EPA HHTV data to toxval from toxval_source

```
toxval.load.epa_hhtv(
  toxval.db,
  source.db,
  log = FALSE,
  remove_null_dtxsid = TRUE
)
```

Arguments

```
toxval.load.epa_ow_npdwr
```

Loading EPA OW NPDWR to toxval from toxval_source

Description

Loading EPA OW NPDWR to toxval from toxval_source

Usage

```
toxval.load.epa_ow_npdwr(
  toxval.db,
  source.db,
  log = FALSE,
  remove_null_dtxsid = TRUE
)
```

Arguments

toxval.db The database version to use

source.db The source database

log If TRUE, send output to a log file

remove_null_dtxsid

If TRUE, delete source records without curated DTXSID value

```
toxval.load.epa_ow_nrwqc_hhc
```

Loading EPA OW NRWQC-HHC to toxval from toxval_source

Description

Loading EPA OW NRWQC-HHC to toxval from toxval_source

toxval.load.generic 67

Usage

```
toxval.load.epa_ow_nrwqc_hhc(
  toxval.db,
  source.db,
  log = FALSE,
  remove_null_dtxsid = TRUE
)
```

Arguments

toxval.db The database version to use

source.db The source database

log If TRUE, send output to a log file

remove_null_dtxsid

If TRUE, delete source records without curated DTXSID value

toxval.load.generic

Generic structure for loading to toxval from toxval_source

Description

Generic structure for loading to toxval from toxval_source

Usage

```
toxval.load.generic(
  toxval.db,
  source.db,
  log = FALSE,
  remove_null_dtxsid = TRUE
)
```

Arguments

toxval.db The database version to use

source.db The source database

log If TRUE, send output to a log file

remove_null_dtxsid

If TRUE, delete source records without curated DTXSID value

68 toxval.load.gestis.dnel

```
toxval.load.genetox.all
```

Load the Genetox data from Grace

Description

Load the Genetox data from Grace

Usage

```
toxval.load.genetox.all(
  toxval.db,
  source.db,
  sys.date = "2021-09-10",
  verbose = FALSE
)
```

Arguments

```
toxval.db The database to use.

source.db The source database to use.

sys.date The input file version

verbose If TRUE output debug information
```

toxval.load.gestis.dnel

Load GESTIS DNEL data from toxval_source to toxval

Description

Load GESTIS DNEL data from toxval_source to toxval

```
toxval.load.gestis.dnel(
  toxval.db,
  source.db,
  log = FALSE,
  remove_null_dtxsid = TRUE
)
```

toxval.load.hawc 69

Arguments

toxval.db The database version to use source.db The source database log If TRUE, send output to a log file

remove_null_dtxsid

If TRUE, delete source records without curated DTXSID value

toxval.load.hawc

Load HAWC from toxval_source to toxval

Description

Load HAWC from toxval_source to toxval

Usage

```
toxval.load.hawc(toxval.db, source.db, log = FALSE, remove_null_dtxsid = TRUE)
```

Arguments

toxval.db The database version to use source.db The source database log If TRUE, send output to a log file remove_null_dtxsid

If TRUE, delete source records without curated DTXSID value

```
toxval.load.hawc_pfas_150
```

Load HAWC PFAS 150 from toxval_source to toxval

Description

Load HAWC PFAS 150 from toxval_source to toxval

```
toxval.load.hawc_pfas_150(
  toxval.db,
  source.db,
  log = FALSE,
  remove_null_dtxsid = TRUE
)
```

70 toxval.load.healthcanada

Arguments

toxval.db The version of toxval into which the tables are loaded.

source.db The version of toxval_source from which the tables are loaded.

log If TRUE, send output to a log file

remove_null_dtxsid

If TRUE, delete source records without curated DTXSID value

```
toxval.load.hawc_pfas_430
```

Load HAWC PFAS 430 from toxval_source to toxval

Description

Load HAWC PFAS 430 from toxval_source to toxval

Usage

```
toxval.load.hawc_pfas_430(
  toxval.db,
  source.db,
  log = FALSE,
  remove_null_dtxsid = TRUE
)
```

Arguments

toxval.db The version of toxval into which the tables are loaded.

source.db The version of toxval_source from which the tables are loaded.

log If TRUE, send output to a log file

remove_null_dtxsid

If TRUE, delete source records without curated DTXSID value

toxval.load.healthcanada

Load Health Canada data from toxval_source to toxval

Description

Generic structure for laoding to toxval from toxval_source

toxval.load.heast 71

Usage

```
toxval.load.healthcanada(
  toxval.db,
  source.db,
  log = FALSE,
  remove_null_dtxsid = TRUE
)
```

Arguments

toxval.db The database version to use

source.db The source database

log If TRUE, send output to a log file

remove_null_dtxsid

If TRUE, delete source records without curated DTXSID value

toxval.load.heast

Load the HEAST data from toxval_source to toxval

Description

Load the HEAST data from toxval_source to toxval

Usage

```
toxval.load.heast(toxval.db, source.db, log = FALSE, remove_null_dtxsid = TRUE)
```

Arguments

toxval.db The database version to use

source.db The source database

log If TRUE, send output to a log file

remove_null_dtxsid

If TRUE, delete source records without curated DTXSID value

72 toxval.load.hpvis

toxval.load.hess

Load HESS data to ToxVal

Description

Load HESS data to ToxVal

Usage

```
toxval.load.hess(toxval.db, source.db, log = FALSE, remove_null_dtxsid = TRUE)
```

Arguments

toxval.db The database version to use

source.db The source database

log If TRUE, send output to a log file

 $remove_null_dtxsid$

If TRUE, delete source records without curated DTXSID value

toxval.load.hpvis

Load HPVIS from toxval_source to toxval

Description

Load HPVIS from toxval_source to toxval

Usage

```
toxval.load.hpvis(toxval.db, source.db, log = FALSE, remove_null_dtxsid = TRUE)
```

Arguments

toxval.db The database version to use

source.db The source database

log If TRUE, send output to a log file

remove_null_dtxsid

If TRUE, delete source records without curated DTXSID value

toxval.load.initial 73

toxval.load.initial Delete the contents of the toxval database

Description

Delete the contents of the toxval database

Usage

```
toxval.load.initial(toxval.db)
```

Arguments

toxval.db The version of toxval from which the data is deleted.

toxval.load.iris

Load IRIS source from toxval_source to toxval

Description

Load IRIS source from toxval_source to toxval

Usage

```
toxval.load.iris(toxval.db, source.db, log = FALSE, remove_null_dtxsid = TRUE)
```

Arguments

toxval.db The version of toxval into which the tables are loaded.

source.db The source database to use.

If TRUE, send output to a log file log

remove_null_dtxsid

74 toxval.load.niosh

 ${\it toxval.load.mass_mmcl} \begin{tabular}{ll} Load\ the\ Mass.\ Drinking\ Water\ Standards\ data\ from\ toxval_source\ to\ toxval \end{tabular}$

Description

Load the Mass. Drinking Water Standards data from toxval_source to toxval

Usage

```
toxval.load.mass_mmcl(
  toxval.db,
  source.db,
  log = FALSE,
  remove_null_dtxsid = TRUE
)
```

Arguments

toxval.db The database version to use

source.db The source database

log If TRUE, send output to a log file

remove_null_dtxsid

If TRUE, delete source records without curated DTXSID value

toxval.load.niosh

Load NIOSH from toxval_source to toxval

Description

Load NIOSH from toxval_source to toxval

Usage

```
toxval.load.niosh(toxval.db, source.db, log = FALSE, remove_null_dtxsid = TRUE)
```

Arguments

toxval.db The database version to use

source.db The source database

log If TRUE, send output to a log file

remove_null_dtxsid

toxval.load.ntp.pfas 75

toxval.load.ntp.pfas Load NTP PFAS data from toxval_source to toxval Generic structure for laoding to toxval from toxval_source

Description

Load NTP PFAS data from toxval_source to toxval Generic structure for laoding to toxval from toxval_source

Usage

```
toxval.load.ntp.pfas(
  toxval.db,
  source.db,
  log = FALSE,
  remove_null_dtxsid = TRUE
)
```

Arguments

toxval.db The database version to use

source.db The source database

log If TRUE, send output to a log file

remove_null_dtxsid

If TRUE, delete source records without curated DTXSID value

toxval.load.opp

Load EPA OPP data to toxval from toxval_source

Description

Load EPA OPP data to toxval from toxval_source

Usage

```
toxval.load.opp(toxval.db, source.db, log = FALSE, remove_null_dtxsid = TRUE)
```

Arguments

toxval.db The database version to use

source.db The source database

log If TRUE, send output to a log file

remove_null_dtxsid

76 toxval.load.ow_dwsha

```
toxval.load.osha_air_limits

Load the osha_air_limits (old ACToR - flex)data from toxval sourcedb

to toxval
```

Description

Load the osha_air_limits (old ACToR - flex)data from toxval sourcedb to toxval

Usage

```
toxval.load.osha_air_limits(toxval.db, source.db, log = F)
```

Arguments

toxval.db The database version to use

source.db The source database

log If TRUE, send output to a log file

Description

Load the ow_dwsha data from toxval_source to toxval

Usage

```
toxval.load.ow_dwsha(
  toxval.db,
  source.db,
  log = FALSE,
  remove_null_dtxsid = TRUE
)
```

Arguments

toxval.db The database version to use

source.db The source database

log If TRUE, send output to a log file

remove_null_dtxsid

toxval.load.penn 77

toxval.load.penn

Load Penn data from toxval_source to toxval

Description

Load Penn data from toxval_source to toxval

Usage

```
toxval.load.penn(toxval.db, source.db, log = FALSE, remove_null_dtxsid = TRUE)
```

Arguments

toxval.db The version of toxval into which the tables are loaded.

source.db The source database to use.

log If TRUE, send output to a log file

remove_null_dtxsid

If TRUE, delete source records without curated DTXSID value

```
toxval.load.penn_dep_mscs
```

Load the penn_dep_mscs data from toxval_source to toxval

Description

Load the penn_dep_mscs data from toxval_source to toxval

Usage

```
toxval.load.penn_dep_mscs(
  toxval.db,
  source.db,
  log = FALSE,
  remove_null_dtxsid = TRUE
)
```

Arguments

toxval.db The database version to use

source.db The source database

log If TRUE, send output to a log file

remove_null_dtxsid

```
toxval.load.pfas_150_sem_v2

Load pfas_150_sem from toxval_source to toxval
```

Description

Load pfas_150_sem from toxval_source to toxval

Usage

```
toxval.load.pfas_150_sem_v2(
  toxval.db,
  source.db,
  log = FALSE,
  remove_null_dtxsid = TRUE
)
```

Arguments

```
toxval.load.postprocess
```

Do all of the post-processing steps for a source

Description

Do all of the post-processing steps for a source

Usage

```
toxval.load.postprocess(
  toxval.db,
  source.db,
  source,
  do.convert.units = FALSE,
  chem_source,
  subsource = NULL,
  remove_null_dtxsid = TRUE
)
```

toxval.load.pprtv.cphea 79

Arguments

toxval.db The database version to use source.db The source database name

source The source name

do.convert.units

If TRUE, convert units, mainly from ppm to mg/kg-day. This code is not de-

bugged

subsource The specific subsource to process, if desired (Default: NULL)

remove_null_dtxsid

If TRUE, delete source records without curated DTXSID value

toxval.load.pprtv.cphea

Load PPRTV CPHEA from toxval_source to toxval

Description

Load PPRTV CPHEA from toxval_source to toxval

Usage

```
toxval.load.pprtv.cphea(
  toxval.db,
  source.db,
  log = FALSE,
  remove_null_dtxsid = TRUE
)
```

Arguments

toxval.db The database version to use

source.db The source database

log If TRUE, send output to a log file

remove_null_dtxsid

80 toxval.load.skin.eye

toxval.load.rsl

Load the RSL data from source db to toxval - the source database needs to be updated periodically

Description

Load the RSL data from source db to toxval - the source database needs to be updated periodically

Usage

```
toxval.load.rsl(toxval.db, source.db, log = FALSE, remove_null_dtxsid = TRUE)
```

Arguments

toxval.db The database version to use

source.db The source database

log If TRUE, send output to a log file

remove_null_dtxsid

If TRUE, delete source records without curated DTXSID value

toxval.load.skin.eye Load the Skin eye data

Description

Load the Skin eye data

Usage

```
toxval.load.skin.eye(toxval.db, source.db, verbose = FALSE)
```

Arguments

toxval.db Database version

verbose if TRUE, print diagnostic messages along the way

```
toxval.load.source_chemical
```

Perform the DSSTox mapping

Description

Perform the DSSTox mapping

Usage

```
toxval.load.source_chemical(
  toxval.db,
  source.db,
  source = NULL,
  verbose = TRUE,
  remove_null_dtxsid = TRUE
)
```

Arguments

```
toxval.db The version of toxvaldb to use.

source.db The source database version

source The source to update for

verbose If TRUE, print out extra diagnostic messages

remove_null_dtxsid

If TRUE, delete source records without curated DTXSID value
```

toxval.load.species Load the species table

Description

Load the species table

Usage

```
toxval.load.species(toxval.db, date_string = "2023-05-18")
```

Arguments

toxval.db The version of toxval into which the tables are loaded.

date_string The date string for the dictionary files

82 toxval.load.toxrefdb2.1

toxval.load.test

Load TEST data from toxval_source to toxval

Description

Load TEST data from toxval_source to toxval

Usage

```
toxval.load.test(toxval.db, source.db, log = FALSE, remove_null_dtxsid = TRUE)
```

Arguments

toxval.db The database version to use source.db The source database

log If TRUE, send output to a log file

remove_null_dtxsid

If TRUE, delete source records without curated DTXSID value

toxval.load.toxrefdb2.1

Load ToxRefdb data to toxval

Description

Load ToxRefdb data to toxval

Usage

```
toxval.load.toxrefdb2.1(
  toxval.db,
  source.db,
  log = FALSE,
  remove_null_dtxsid = TRUE
)
```

Arguments

toxval.db The database version to use

source.db The source database

log If TRUE, send output to a log file

remove_null_dtxsid

toxval.load.usgs_hbsl 83

Description

Load the usgs_hbsl (old ACToR - flex)data from toxval source db to toxval

Usage

```
toxval.load.usgs_hbsl(toxval.db, source.db, log = F)
```

Arguments

toxval.db The database version to use

source.db The source database

log If TRUE, send output to a log file

toxval.load.ut_hb Load the uterotophic and Hershberger data

Description

Load the uterotophic and Hershberger data

Usage

```
toxval.load.ut_hb(toxval.db, source.db, log = FALSE, remove_null_dtxsid = TRUE)
```

Arguments

toxval.db The database version to use

source.db The source database

log If TRUE, send output to a log file

remove_null_dtxsid

Description

Load the who_ipcs data from toxval source db to toxval

Usage

```
toxval.load.who_ipcs(
  toxval.db,
  source.db,
  log = FALSE,
  remove_null_dtxsid = TRUE
)
```

Arguments

```
toxval.load.who_jecfa_adi
```

Load WHO JECFA ADI from toxval_source to toxval

Description

Load WHO JECFA ADI from toxval_source to toxval

Usage

```
toxval.load.who_jecfa_adi(
  toxvaldb,
  source.db,
  log = FALSE,
  remove_null_dtxsid = TRUE
)
```

Arguments

```
source.db The source database
```

log If TRUE, send output to a log file

remove_null_dtxsid

If TRUE, delete source records without curated DTXSID value

toxval.db The database version to use

```
toxval.load.who_jecfa_tox_studies
```

Load WHO JECFA Tox Studies from toxval_source to toxval

Description

Load WHO JECFA Tox Studies from toxval_source to toxval

Usage

```
toxval.load.who_jecfa_tox_studies(
  toxval.db,
  source.db,
  log = FALSE,
  remove_null_dtxsid = TRUE
)
```

Arguments

toxval.db The database version to use

source.db The source database

log If TRUE, send output to a log file

remove_null_dtxsid

If TRUE, delete source records without curated DTXSID value

toxval.set.mw

Set the molecular weight in the toxval table, for use in unit conversions

Description

Set the molecular weight in the toxval table, for use in unit conversions

Usage

```
toxval.set.mw(toxval.db, source = NULL, subsource = NULL)
```

86 toxvaldb.view

Arguments

toxval.db The database version to use

source The source subsource The subsource

toxval.summary.stats Generate summary statistics on the toxval database

Description

Generate summary statistics on the toxval database

Usage

```
toxval.summary.stats(toxval.db)
```

Arguments

toxval.db The version of toxval into which the tables are loaded.

toxvaldb.view Produce a view of the ToxValDB Data

Description

'toxvaldb.view' Produces a view for ToxValDB by merging specified tables

Usage

```
toxvaldb.view(toxval.db, user, password, count = 10)
```

Arguments

toxval.db Database version

user The username for the MySQL database. The database instance is hard-coded in

the function setDBConn().

password The user's MySQL database password.

count If count>0, only select this number of records from each source, used for debug-

ging

Value

Write a file with the results: data/view/ToxValDB View toxval.db Sys.Date().xlsx

toxval_type.species.mismap

Find species and toxval_type mismaps, e.g. species other than human fro RfD, RfC, cancer sloper, MSL, etc.

Description

Find species and toxval_type mismaps, e.g. species other than human fro RfD, RfC, cancer sloper, MSL, etc.

Usage

```
toxval_type.species.mismap(toxval.db)
```

Arguments

toxval.db Database version

source The source to be updated

Value

Write a file with the results

%>%

Pipe operator

Description

```
See magrittr::%>% for details.
```

Usage

lhs %>% rhs

Arguments

1hs A value or the magrittr placeholder.

rhs A function call using the magrittr semantics.

Value

The result of calling 'rhs(lhs)'.

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