toxvaldb09

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```
Type Package
Title Builds the ToxValDB V9.2 Database
Version 1.0.1
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Description
      ToxValDB is a database containing quantitative records form in vivo toxicologye studies from
      many sources (46 for this release). The database has 2 main parts - toxval_source containing
      source data in separate tables, and the main toxval schema which combines data from multi-
      into a single format. Data is read from files or other databses into toxval_sources and then
      pulled into toxval where terms are converted to standard values. The ToxValDB SOPs de-
      scribe in more
      detail how to run the code.
Imports DBI,
     RMySQL,
     openxlsx,
      dplyr,
      tidyr,
      stringr,
      tibble,
     janitor,
     logr
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```

R topics documented:

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cas_checkSum

Check CAS RN validity via checksum method

Description

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

Usage

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

Arguments

 \times 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.

6 chem.check

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.

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))</pre>
```

chem.check

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

chem.check.v2 7

Usage

```
chem.check(
  res0,
  name.col = "name",
  casrn.col = "casrn",
  source = NULL,
  verbose = F
)
```

Arguments

res0	The data frame in which chemicals names and CASRN will be replaced
name.col	The column name that contains the chemical names
casrn.col	The column name that contains the CARN values
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=c

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 chem-
	check.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, source = NULL, verbose = F)
```

Arguments

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

```
clean.last.character
```

Clean unneeded characters from the end of a string

Description

Clean unneeded characters from the end of a string

Usage

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

Arguments

Х

String to be cleaned

Value

The cleaned string

```
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

clowder_document_list 9

```
clowder_document_list
```

Get a listing of all of the documents in clowder and link back to information in dev_toxval_v8

Description

Get a listing of all of the documents in clowder and link back to information in dev_toxval_v8

Usage

```
clowder_document_list(db = "dev_toxval_v8")
```

Arguments

db

The version of toxval into which the source is loaded.

clowder_id_prep.v3 Organize the clowder_id and document_name information

Description

Organize the clowder_id and document_name information

Usage

```
clowder_id_prep.v3(db = "dev_toxval_v9")
```

Arguments

db

The version of toxval into which the source is loaded.

File from clowder linking clowder_ids to document_names, generated by Taylor Wall clowder_doc_maps_20220608.xlsx

10 ecotox.datahub.to.file

contains

Find out if one string contains another

Description

Find out if one string contains another

Usage

```
contains(x, query, verbose = F)
```

Arguments

x The string to be searched in

query the second string

verbose if TRUE, the two strings are printed

Value

if x contains query, return TRUE, FALSE otherwise

```
ecotox.datahub.to.file
```

Extract ECOTOX from the datahub to a file

Description

Extract ECOTOX from the datahub to a file

Usage

```
ecotox.datahub.to.file(toxval.db, verbose = T, do.load = F)
```

Arguments

 ${\tt toxval.db} \qquad {\tt The\ version\ of\ toxval\ into\ which\ the\ tables\ are\ loaded}.$

verbose Whether the loaded rows should be printed to the console.

do.load If TRUE, load the data from the input file and put into a global variable

export.all.by.source 11

```
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)
```

Arguments

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.all.with.references
```

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.all.with.references(toxval.db, dir = "../export/", file.name = NA)
```

Arguments

	D . 1
t.oxval.db	Database version

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

exported

human_eco Either 'human health' or 'eco'

Value

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

export.dsstox

Export the DSSTox chemical table

Description

Export the DSSTox chemical table

Usage

```
export.dsstox()
```

```
export.final.params
```

Export the final values for the character params (e.g. toxval_type).

Description

Export the final values for the character params (e.g. toxval_type).

Usage

```
export.final.params(toxval.db)
```

Arguments

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

```
export.missing.rac.by.source
```

Export the rows with a missing risk_assessment_class

Description

Export the rows with a missing risk_assessment_class

Usage

```
export.missing.rac.by.source(toxval.db, source)
```

Arguments

toxval.db Database version

source The source to be processed

Value

writes an Excel file with the name ./qc_export/toxval_missing_risk_assessment_class_Sys.Date().xlsx"

export.source_chemical

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```
export.source_chemical
```

Export the source chemical table

Description

Export the source chemical table

Usage

```
export.source_chemical(db)
```

Arguments

db

The name of the database String to be cleaned

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

Fill the chemical table

Description

Fill the chemical table

Usage

```
## S3 method for class 'chemical.by.source'
fill(toxval.db, source, verbose = T)
```

Arguments

toxval.db The version of toxvaldb to use.

source The source to be used

verbose If TRUE, print out extra diagnostic messages

14 fill.toxval.defaults

```
fill.chemical_source_index
```

 $Load\ the\ chemical_source_index\ table.$

Description

Load the chemical_source_index table.

Usage

```
## S3 method for class 'chemical_source_index'
fill(db)
```

Arguments

db

The version of toxval_source into which the source is loaded.

```
fill.toxval.defaults
```

Set Toxval Defaults

Description

Set Toxval Defaults

Usage

```
## S3 method for class 'toxval.defaults'
fill(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

```
## S3 method for class 'toxval.defaults.global.by.source'
fill(toxval.db, source)
```

Arguments

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

source The source to be fixed

```
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, fill.toxval_fix = T)
```

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.casrn

Fix a CASRN that has one of several problems

Description

Fix a CASRN that has one of several problems

Usage

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

Arguments

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

Value

the fixed CASRN

```
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)
```

Arguments

toxval.db The version of toxvaldb to use.

source THe source to be fixed

fix.empty.by.source 17

```
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)
```

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

Description

Set all empty cells in record_source to '-'

Usage

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

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_method.and.form.by.source

Exposure Method temporary fix to add Exposure Form
```

Description

Exposure Method temporary fix to add Exposure Form

Usage

```
fix.exposure_method.and.form.by.source(toxval.db, source)
```

Arguments

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

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)
```

Arguments

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

source The source to be processes

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, reset = T)
```

Arguments

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

source The source to be fixed

reset If TRUE, reset all values to 'not specified' before processing all records in the

source

Value

The database will be altered

```
fix.non_ascii.v2 Flag and fix non-ascii characters in the database
```

Description

Flag and fix non-ascii characters in the database

Usage

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

Arguments

df The dataframe to be processed

The source to be fixed

Value

The dataframe with non ascii characters replaced with cleaned versions

```
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)
```

Arguments

toxval.db The version of toxvaldb to use.

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

```
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 = NULL, reset = T)
```

Arguments

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

source The source to be fixed

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

Value

The database will be altered

```
fix.risk_assessment_class.all.source
```

Fix the risk assessment class for all source.

Description

Fix the risk assessment class for all source.

Usage

```
fix.risk_assessment_class.all.source(toxval.db, restart = T)
```

Arguments

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

restart If TRUE, delete all values and start from scratch

```
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, restart = T)
```

Arguments

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

source The source to be updated

restart If TRUE, delete all values and start from scratch

fix.species.v2

```
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, ignore = FALSE)
```

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

ignore If TRUE allow missing values to be ignored

Value

The database will be altered

```
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, date_string = "2022-05-25")
```

Arguments

toxval.db The version of the database to use

source The source to be fixed

date_string The date version of the dictionary

fix.strain.v2

fix.strain.v2

Set the strain information in toxval

Description

Set the strain information in toxval

Usage

```
fix.strain.v2(toxval.db, source, date_string = "2022-05-25")
```

Arguments

toxval.db The version of the database to use

source The source to be fixed

date_string The date of hte latest dictinary version

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

Usage

```
fix.units.by.source(toxval.db, source, do.convert.units = F)
```

24 get.cid.list.toxval

Arguments

toxval.db The version of toxvaldb to use.

source Source to be fixed

do.convert.units

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

generate.originals Duplicate any columns with '_original' Set Toxval Defaults

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

```
get.cid.list.toxval
```

Get chemical ids for many given CASRN/Chemical name pairs

Description

Get chemical ids for many given CASRN/Chemical name pairs

Usage

```
get.cid.list.toxval(toxval.db, chemical.list, source, verbose = F)
```

Arguments

toxval.db The version of toxval that the chemical id is pulled from.

chemical.list

A 2-column dataframe of CAS Registry Numbers and chemical names.

source The source of the chemical data

verbose If TRUE, print out extra diagnostic messages

getPSQLDBConn 25

Value

A 3-column dataframe of CAS Registry Numbers, chemical names, and associated chemical IDs.

getPSQLDBConn

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

Description

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

Usage

```
getPSQLDBConn()
```

Value

print the database connection information

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

26 import.source.info

import.driver

Function to run all import scripts to fill toxval_source

Description

Function to run all import scripts to fill toxval_source

Usage

```
import.driver(
   db = "res_toxval_source_v5",
   chem.check.halt = FALSE,
   do.clean = FALSE
)
```

Arguments

db The version of toxval_source into which the source is loaded.

do.clean If TRUE, delte data from all tables before reloading

chem.chek.halt

If TRUE and there are bad chemical names or casrn, stop to look at the results in indir/chemcheck.xlsx

import.source.info Load Source Info into toxval. The information is in the file ./dictionary/source_in_2020_aug_17.xlsx

Description

Load Source Info into toxval. The information is in the file ./dictionary/source_in_2020_aug_17.xlsx

Usage

```
import.source.info(toxval.db)
```

Arguments

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

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

Load Source Info for each source into toxval The information is in the file ~/dictionary/source_in_2020_aug_17.xlsx

Description

Load Source Info for each source into toxval The information is in the file ~/dictionary/source_in_2020_aug_17.xlsx

Usage

```
import.source.info.by.source(toxval.db, source = NULL)
```

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

```
import_atsdr_pfas_2021_source
```

Load ATSDR PFAS 2021 Source into toxval_source

Description

Load ATSDR PFAS 2021 Source into toxval_source

Usage

```
import_atsdr_pfas_2021_source(db, chem.check.halt = F)
```

Arguments

db The version of toxval_source into which the source is loaded.

chem.check.halt

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

indir The path for all the input xlsx files ./atsdr_pfas_2021/atsdr_pfas_2021_files

28 import_atsdr_source

```
import_atsdr_pfas_source
```

Load ATSDR PFAS Source files into toxval_source

Description

Load ATSDR PFAS Source files into toxval_source

Usage

```
import_atsdr_pfas_source(
   db,
   infile1 = "ATSDR_Perfluoroalkyls_Inhalation.xlsx",
   infile2 = "ATSDR_Perfluoroalkyls_Oral.xlsx",
   infile3 = "ATSDR_PFOA_Inhalation.xlsx",
   infile4 = ".ATSDR_PFOA_Oral.xlsx",
   infile5 = "ATSDR_PFOS_Oral.xlsx",
   chem.check.halt = F
)
```

Arguments

db	The version of toxval_source into which the source is loaded.	
infile1	$The input file \ ./atsdr_pfas/atsdr_pfas_files/ATSDR_Perfluoroalkyls_Inhalation.xlsx$	
infile2	The input file ./atsdr_pfas/atsdr_pfas_files/ATSDR_Perfluoroalkyls_Oral.xlsx	
infile3	The input file ./atsdr_pfas/atsdr_pfas_files/ATSDR_PFOA_Inhalation.xlsx	
infile4	The input file ./atsdr_pfas/atsdr_pfas_files/ATSDR_PFOA_Oral.xlsx	
infile5	The input file ./atsdr_pfas/atsdr_pfas_files/ATSDR_PFOS_Oral.xlsx	
chem.check.halt		

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

```
import_atsdr_source
```

Load atsdr Source into toxval_source

Description

Load atsdr Source into toxval_source

Usage

```
import_atsdr_source(
   db,
   infile = "ATSDR_MRLs_2020_Sept2020_Temp.xlsx",
   chem.check.halt = F
)
```

Arguments

```
db The version of toxval_source into which the source is loaded.

infile The input file /atsdr/atsdr_files/ATSDR_MRLs_2020_Sept2020_Temp.xls chem.check.halt
```

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

```
import_caloehha_source
```

Load caloehha Source file into toxval_source The raw data can be exported as an Excel sheet from the web site https://oehha.ca.gov/chemicals, selecting the link "Export database as .CSV file"

Description

This method parses that file and prepares for loading into toxval source

Usage

```
import_caloehha_source(
   db,
   infile = "OEHHA-chemicals_2022-06-22T13-42-44.xlsx",
   chem.check.halt = F
)
```

Arguments

db The version of toxval_source into which the source is loaded.

infile The input file ="../caloehha/caloehha_files/OEHHA-chemicals_2018-10-30T08-

50-47.xlsx",

chem.check.halt

If TRUE and there are problems with chemicals CASRN checks, halt the program

Description

Load chiu Source into dev_toxval_source_v3. Data from the Chiu et al. paper on RfD values

Usage

```
import_chiu_source(
   db,
   infile = "Full_RfD_databaseQAed-FINAL.xlsx",
   chem.check.halt = F
)
```

Arguments

db The version of toxval_source into which the source is loaded.

 $\verb|infile| The input file ./chiu/chiu_files/Full_RfD_databaseQAed-FINAL.xlsx| \\$

chem.check.halt

If TRUE and there are bad chemical names or casrn, stop to look at the results in indir/chemcheck.xlsx

```
import_copper_source
```

Load copper manufacturers Source into toxval_source

Description

Load copper manufacturers Source into toxval_source

Usage

```
import_copper_source(
   db,
   infile = "Copper Data Entry - Final.xlsx",
   chem.check.halt = F
)
```

Arguments

db The version of toxval_source into which the source is loaded.

infile The input file ./copper/copper_files/Copper Data Entry - Final.xlsx

chem.check.halt

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

import_cosmos_source 31

```
import_cosmos_source
```

Load cosmos Source files into toxval_source

Description

Load cosmos Source files into toxval_source

Usage

```
import_cosmos_source(
   db,
   infile1 = "COSMOS_DB_v1_export_2016_04_02_study_data.xlsx",
   infile2 = "COSMOS_DB_v1_export_2016_04_02_cosmetics_inventory.xlsx",
   chem.check.halt = F
)
```

Arguments

db The version of toxval_source into which the source is loaded.

 $\verb|infile1| The input file ./cosmos/cosmos_files/COSMOS_DB_v1_export_2016_04_02_study_data.xlsx| \\$

infile2 The input file ./cosmos/cosmos_files/COSMOS_DB_v1_export_2016_04_02_cosmetics_inventory.xlsx

chem.check.halt

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

```
import_dod_ered_source
```

Load dod Source into toxval_source

Description

Load dod Source into toxval_source

Usage

```
import_dod_ered_source(
   db,
   infile = "USACE_ERDC_ERED_database_12_07_2018.xlsx",
   chem.check.halt = F
)
```

Arguments

db The version of toxval_source into which the source is loaded.

infile The input file ./dod/dod_files/USACE_ERDC_ERED_database_12_07_2018.xlsx
chem.check.halt

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

Description

Load DOD MEG to toxval_source. The file to be loaded are in ./dod/dod_files

Usage

```
import_dod_source(db, chem.check.halt = F)
```

Arguments

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

Description

Load doe_benchmarks Source into toxval_source

Usage

```
import_doe_benchmarks_source(
   db,
   infile = "DOE_Wildlife_Benchmarks_1996.xlsx",
   chem.check.halt = F
)
```

Arguments

db The version of toxval_source into which the source is loaded.

infile The input file ./doe_benchmarks/doe_benchmarks_files/DOE_Wildlife_Benchmarks_1996.xlsx
chem.check.halt

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

import_doe_source 33

```
import_doe_source Load DOE Source into toxval_source
```

Description

Load DOE Source into toxval_source

Usage

```
import_doe_source(db, infile = "Revision_29.xlsx", chem.check.halt = F)
```

Arguments

db The version of toxval_source into which the source is loaded.
infile The input file ./doe/doe_files/Revision_29.xlsx

chem.check.halt

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

```
import_echa_echemportal_api_source
Load ECHA echemportal api Source into toxval_source
```

Description

Load ECHA echemportal api Source into toxval_source

Usage

```
import_echa_echemportal_api_source(
   db,
   filepath = "echa_echemportal_api/echa_echemportal_api_files",
   chem.check.halt = T
)
```

Arguments

db The version of toxval_source into which the source is loaded.

 $\label{lem:check-lem:check-lem:check} The path for all the input xlsx files ./echa_echemportal_api/echa_echemportal_api_files \\ \texttt{chem.check.halt}$

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

34 import_efsa_source

```
import_efsa2_source
```

Load efsa2 Source into toxval_source

Description

Load efsa2 Source into toxval_source

Usage

```
import_efsa2_source(
   db,
   infile = "EFSA_combined_new 2022-07-19.xlsx",
   chem.check.halt = F
)
```

Arguments

db The version of toxval_source into which the source is loaded.

infile The input file /efsa2/efsa2_files/merge2/EFSA_combined_new.xlsx
chem.check.halt

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

import_efsa_source Process the raw excel files downloaded from EFSA version3(March 27 2020) To get the files, go to the web site https://zenodo.org/record/3693783#.XrsBMmhKjIU. At the bottom are links to a set of Excel files - download all of them into the next version V3, convert the xlsx files to csv since the xlsx files when read in R converts all symbols/special characters to certain unicode values (space to '_x0020_'). while reading the original xlsx files into R it was unsuccessful to convert enconding to UTF-8, also tried converting using stringi. Only workaround was by converting the downloaded files to csv and using the csv files as input source.

Description

Process the raw excel files downloaded from EFSA version3(March 27 2020) To get the files, go to the web site https://zenodo.org/record/3693783#.XrsBMmhKjIU. At the bottom are links to a set of Excel files - download all of them into the next version V3, convert the xlsx files to csv since the xlsx files when read in R converts all symbols/special characters to certain unicode values (space to '_x0020_'). while reading the original xlsx files into R it was unsuccessful to convert enconding to UTF-8, also tried converting using stringi. Only workaround was by converting the downloaded files to csv and using the csv files as input source.

Usage

```
import_efsa_source(db, chem.check.halt = F)
```

Arguments

```
db The version of toxval_source into which the source is loaded. chem.check.halt
```

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

```
import_envirotox_source
```

Load EnviroTox.V2 Source data into toxval_source

Description

Load EnviroTox.V2 Source data into toxval_source

Usage

```
import_envirotox_source(
  db,
  infile = "envirotox_taxonomy clean casrn.xlsx",
  chem.check.halt = F
)
```

Arguments

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

infile The input file /envirotox/envirotox_files/envirotox_taxonomy.xlsx
chem.check.halt

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

Description

Load the FLEX data (old ACToR data) from files to toxval source. This will load all Excel file in the folder ACToR replacements/

Usage

```
import_flex_source(
   db,
   filepath = "ACTOR replacements",
   verbose = F,
   chem.check.halt = F,
   do.clean = F
```

Arguments

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

filepath The path for all the input xlsx files ./ACToR replacements

verbose Whether the loaded rows should be printed to the console.

chem.check.halt

If TRUE and there are problems with chemicals CASRN checks, halt the program

do.clean If true, remove data for these sources before reloading

Description

Load HAWC PFAS 150 Source into toxval_source

Usage

```
import_hawc_pfas_150_source(
   db,
   infile1 = "hawc_pfas_150_raw3.xlsx",
   infile2 = "hawc_pfas_150_doses3.xlsx",
   infile3 = "hawc_pfas_150_groups3.xlsx",
   chem.check.halt = F
)
```

Arguments

db	The version of toxval_source into which the source is loaded.
infile1	The input file ./hawc_pfas/hawc_pfas_files/hawc_pfas_150_raw3.xlsx , extracted from https://hawcprd.epa.gov , assessment name - PFAS 150 (2021) and assessment id - 100500085. Data extraction using HawcClient and extraction script hawc_pfas_150.py
infile2	The input file ./hawc_pfas/hawc_pfas_files/hawc_pfas_150_doses3.xlsx

```
infile3 The input file ./hawc_pfas/hawc_pfas_files/hawc_pfas_150_groups3.xlsx
chem.check.halt
```

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

Description

Load HAWC PFAS 430 Source into toxval_source

Usage

```
import_hawc_pfas_430_source(
   db,
   infile1 = "hawc_pfas_430_raw3.xlsx",
   infile2 = "hawc_pfas_430_doses3.xlsx",
   infile3 = "hawc_pfas_430_groups3.xlsx",
   chem.check.halt = T
)
```

Arguments

db	The version of toxval_source into which the source is loaded.	
infile1	The input file ./hawc_pfas_430/hawc_pfas_430_files/hawc_pfas_430_raw3.xlsx , extracted from https://hawcprd.epa.gov , assessment name - PFAS 430 (2020) and assessment id - 100500256. Data extraction using HawcClient and extraction script hawc_pfas_430.py	
infile2	The input file ./hawc_pfas_430/hawc_pfas_430_files/hawc_pfas_430_doses3.xlsx	
infile3	The input file ./hawc_pfas_430/hawc_pfas_430_files/hawc_pfas_430_groups3.xlsx	
chem.check.halt		

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

```
import_hawc_source Load HAWC Source into toxval_source
```

Description

Note that the different tabs in the input sheet have different names, so these need to be adjusted manually for the code to work. This is a problem wit how the data is stored in HAWC

Usage

```
import_hawc_source(
   db,
   infile1 = "hawc_original_12_06_21.xlsx",
   infile2 = "dose_dict.xlsx",
   chem.check.halt = T
)
```

Arguments

db The version of toxval_source into which the source is loaded.

infile1 The input file ./hawc/hawc_files/hawc_original_12_06_21.xlsx

infile2 The input file ./hawc/hawc_files/dose_dict.xlsx

chem.check.halt

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

```
import_health_canada_source
```

Load Health Canada Source Info into toxval_source

Description

Load Health Canada Source Info into toxval_source

Usage

```
import_health_canada_source(
   db,
   infile = "HealthCanada_TRVs_2010_AppendixA v2.xlsx",
   chem.check.halt = T
)
```

Arguments

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

infile The input file ./health_canada/health_canada_files/HealthCanada_TRVs_2010_AppendixAv2.xlsx

chem.check.halt

import_heast_source 39

```
import_heast_source
```

Load HEAST Source into toxval_source

Description

Load HEAST Source into toxval_source

Usage

```
import_heast_source(
   db,
   infile = "EPA_HEAST_Table1_ORNL for loading.xlsx",
   chem.check.halt = T
)
```

Arguments

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

import_hess_source Load HESS Source into toxval_source

Description

Load HESS Source into toxval_source

Usage

```
import_hess_source(
   db,
   infile1 = "hess_6_16_21.xlsx",
   infile2 = "hess_record_urls_from_clowder.xlsx",
   chem.check.halt = T
)
```

Arguments

db The version of toxval_source into which the source is loaded.

infile1 The input file ./hess/hess_files/hess_6_16_21.csv, extracted by Risa Sayre(SCDCD)

infile2 The input file ./hess/hess_files/hess_record_urls_from_clowder.xlsx

chem.check.halt

40 import_iris_source

```
import_hpvis_source
```

Load HPVIS Source Info into toxval_source

Description

Load HPVIS Source Info into toxval_source

Usage

```
import_hpvis_source(db, filepath = "hpvis/hpvis_files", chem.check.halt = T)
```

Arguments

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

filepath The path for all the input xlsx files ./hpvis/hpvis_files

chem.check.halt

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

import_iris_source Load IRIS Source into toxval_source

Description

Load IRIS Source into toxval_source

Usage

```
import_iris_source(
   db,
   infile1 = "IRIS_non_cancer_clean 2020-05-27.xlsx",
   infile2 = "IRIS_cancer_clean 2020-05-27.xlsx",
   chem.check.halt = T
)
```

Arguments

db The version of toxval_source into which the source is loaded.

infile1 The input file ./iris/iris_files/IRIS_non_cancer_clean 2020-05-27.xlsx

infile2 The input file ./iris/iris_files/IRIS_cancer_clean 2020-05-27.xlsx

chem.check.halt

import_lanl_source 41

import_lanl_source Load LANL Source into toxval_source

Description

Load LANL Source into toxval_source

Usage

```
import_lanl_source(db, infile = "ESLs_R3.3.xlsx", chem.check.halt = T)
```

Arguments

db The version of toxval_source into which the source is loaded.

infile The input file ./lanl/lanl_files/ESLs_R3.3.xlsx

chem.check.halt

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

import_niosh_source

Load NIOSH Source into toxval_source

Description

Load NIOSH Source into toxval_source

Usage

```
import_niosh_source(db, infile = "niosh_IDLH_2020.xlsx", chem.check.halt = T)
```

Arguments

db The version of toxval_source into which the source is loaded.

infile The input file ./niosh/niosh_files/niosh_IDLH_2020.xlsx

chem.check.halt

42 import_opp_source

import_oppt_source Load OPPT Source Info into toxval_source

Description

Load OPPT Source Info into toxval_source

Usage

```
import_oppt_source(db, infile = "OPPT_data_20181219.xlsx", chem.check.halt = T)
```

Arguments

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

infile The input file ./oppt/oppt_files/OPPT_data_20181219.xlsx

chem.check.halt

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

import_opp_source Load OPP Source into toxval_source

Description

Load OPP Source into toxval_source

Usage

```
import_opp_source(db, infile = "OPP RfD.xlsx", chem.check.halt = T)
```

Arguments

db The version of toxval_source into which the source is loaded.

infile The input file ./opp/opp_files/OPP RfD.xlsx

chem.check.halt

import_penn_source 43

```
import_penn_source Load Penn Source into toxval_source
```

Description

Load Penn Source into toxval_source

Usage

```
import_penn_source(db, infile = "..enn DEP Table 5a.xlsx", chem.check.halt = T)
```

Arguments

db The version of toxval_source into which the source is loaded.

infile The input file ./penn/penn_files/Penn DEP Table 5a.xlsx
chem.check.halt

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

```
import_pfas_150_sem_source
```

Load PFAS 150 SEM Source data into toxval_source

Description

Load PFAS 150 SEM Source data into toxval_source

Usage

```
import_pfas_150_sem_source(
   db,

infile = "PFAS150 animal study template combined_clearance with DTXSID and CASE chem.check.halt = F
)
```

Arguments

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

infile The input file ./PFAS 150 SEM/PFAS 150 SEM_files/PFAS150 animal study

template combined_clearance with DTXSID and CASRN.xlsx

chem.check.halt

If TRUE and there are problems with chemicals CASRN checks, halt the program

```
import_pfas_summary_pods_source
```

Load PFAS Summary PODs into toxval_source

Description

Load PFAS Summary PODs into toxval_source

Usage

```
import_pfas_summary_pods_source(
   db,
   infile1 = "PFAS 150 Study Level PODs_061920.xlsx",
   infile2 = "CompToxChemicalsDashboard-Batch-Search_2020-07-20_17_18_42.xlsx",
   chem.check.halt = T
)
```

Arguments

```
db The version of toxval_source into which the source is loaded.

infile1 The input file ./PFAS Summary PODs/PFAS Summary PODs_files/PFAS 150
Study Level PODs_061920.xlsx

infile2 The input file ./PFAS Summary PODs/PFAS Summary PODs_files/CompToxChemicalsDashboard-Batch-Search_2020-07-20_17_18_42.xls

chem.check.halt
If TRUE and there are problems with chemicals CASRN checks, halt the program
```

```
import_pprtv_ncea_source
```

Load PPRTV NCEA Source Info into toxval_source

Description

Load PPRTV NCEA Source Info into toxval_source

Usage

```
import_pprtv_ncea_source(
   db,
   csvfile = "../pprtv_ncea/pprtv_ncea_files/dose_reg2.csv",
   scrapepath = "../pprtv_ncea/PPRTV_scrape2020-04-08.xlsx",
   chem.check.halt = F
)
```

Arguments

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

csvfile The input csv file ./pprtv_ncea/pprtv_ncea_files/dose_reg2.csv

scrapepath The path for new_pprtv_ncea_scrape_table file ./pprtv_ncea/PPRTV_scrape2020-

04-08.xlsx

chem.check.halt

If TRUE and there are problems with chemicals CASRN checks, halt the pro-

gram

```
import_pprtv_ornl_source
```

Load PPRTV ORNL Source into toxval_source

Description

Load PPRTV ORNL Source into toxval_source

Usage

```
import_pprtv_ornl_source(
   db,
   infile = "new_PPRTV_ORNL cancer noncancer.xlsx",
   chem.check.halt = F
)
```

Arguments

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

 $\verb|infile| The input file ./pprtv_ornl_files/new_PPRTV_ORNL cancer noncancer.xlsx | chem.check.halt \\$

If TRUE and there are problems with chemicals CASRN checks, halt the program

import_rsl_source Load RSL Source Info into toxval source database

Description

Load RSL Source Info into toxval source database

import_test_source

Usage

```
import_rsl_source(
   db,
   infile1a = "final_rsl_thq_combined_nov21.xlsx",
   infile1b = "final_rsl_subchronic_nov21.xlsx",
   infile2 = "general_info_nov_21.xlsx",
   infile3 = "key_description_nov_21.xlsx",
   chem.check.halt = T
)
```

Arguments

db	The version of toxval into which the source info is loaded.	
infile1a	The input file ./rsl/rsl_files/final_rsl_thq_combined_nov21.xlsx	
infile1b	The input file ./rsl/rsl_files/final_rsl_subchronic_nov21.xlsx	
infile2	The input file ./rsl/rsl_files/general_info_nov_21.xlsx	
infile3	The input file ./rsl/rsl_files/key_description_nov_21.xlsx	
chem.check.halt		

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

import_test_source Load TEST Source data into toxval_source

Description

Load TEST Source data into toxval_source

Usage

```
import_test_source(
   db,
   infile1 = "TEST data.xlsx",
   infile2 = "test_chemicals_invitrodb.csv",
   chem.check.halt = T
)
```

Arguments

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

infile1 The input file ./test/test_files/TEST data.xlsx

infile2 The input file ./test/test_files/test_chemicals_invitrodb.csv to map casrn to names from prod_internal_invitrodb_v3_2.chemical

chem.check.halt

import_wignall_source 47

```
import_wignall_source
```

Load wignall Source data into dev_toxval_source_v2.

Description

Load wignall Source data into dev_toxval_source_v2.

Usage

```
import_wignall_source(
   db,
   infile = "BMD_Results_2014-06-17_reviewed Mar 2018 parsed.xlsx",
   chem.check.halt = T
)
```

Arguments

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

infile The input file ./wignall_files/BMD_Results_2014-06-17_reviewed Mar 2018.xlsx

chem.check.halt

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

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()
```

pfas.by.source

log_message

Function to combine output log with output message

Description

Function to combine output log with output message

Usage

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

Arguments

pfas.by.source

Get the sources with PFAS data

Description

Get the sources with PFAS data

Usage

```
pfas.by.source(db)
```

Arguments

db

The version of toxval into which the source is loaded.

printCurrentFunction 49

```
printCurrentFunction
```

Print the name of the current function

Description

Print the name of the current function

Usage

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

Arguments

```
comment.string
```

An optional string to be printed

runInsert Insert a record into a database. if auto.increment=TRUE, return the

auto incremented primary key of the record. otherwise, return -1

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

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

Value

Returns the database table auto incremented primary key ID

runQuery

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Inserts multiple rows into a database table

Description

Inserts multiple rows into a database table

Usage

```
runInsertTable(mat, table, db, do.halt = T, verbose = F, get.id = T)
```

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

runQuery

Runs a database query and returns a result set

Description

Runs a database query and returns a result set

Usage

```
runQuery(query, db, do.halt = T, verbose = F)
```

Arguments

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

runQuery_psql 51

runQuery_psql

Runs a PSQL database query and returns a result set

Description

Runs a PSQL database query and returns a result set

Usage

```
runQuery_psql(query, db, do.halt = T, verbose = T)
```

Arguments

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

setDBConn

set SQL connection to the database

Description

set SQL connection to the database

Usage

```
setDBConn(server = "ccte-mysql-res.epa.gov", user, password)
```

Arguments

server SQL server on which relevant database lives

user SQL username to access database

password SQL password corresponding to username

set_clowder_id

setPSQLDBConn

set PSQL connection to the database

Description

set PSQL connection to the database

Usage

```
setPSQLDBConn(server, port, user, password)
```

Arguments

server SQL server on which relevant database lives

user SQL username to access database

password SQL password corresponding to username

set_clowder_id

Set the clowder_id and document_name in res

Description

Set the clowder_id and document_name in res

Usage

```
set_clowder_id(res, source)
```

Arguments

res The input dataframe source The data source name

Value

Returns the input dataframe with defaults set

source.size 53

source.size

print out the size of each of the tables in toxval_source

Description

print out the size of each of the tables in toxval_source

Usage

```
source.size(db = "res_toxval_source_v5")
```

Arguments

db

The version of toxval_source into which the source is loaded.

```
source_chemical.duplicates
```

Find duplicated chemicals in the source_chemical table. This will help get rid of records that have been repalced

Description

Find duplicated chemicals in the source_chemical table. THis will help get rid of records that have been repalced

Usage

```
source_chemical.duplicates(db)
```

Arguments

db

The version of toxval into which the tables are loaded.

```
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.process
```

Deal with the process of making the source_chemical information

Description

Deal with the process of making the source_chemical information

Usage

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

Arguments

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

The input dataframe to which chemical information will be added source

The source to process 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 the column containing hte chemical name

If TRUE, write out diagnostic messages

Value

verbose

Returns the original dataframe with a chemical_id appended

```
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 = F
)
```

Arguments

The version of toxval into which the source info is loaded. toxval.db The source database version source.db The dataframe to which the chemical_id sill be added res The name of the source source chem.check.halt If TRUE, stop if there are problems with the chemical mapping The name of the column containing the CASRN casrn.col 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

```
source_prep_and_load

Prep the source data aand load
```

Description

Prep the source data aand load

Usage

```
source_prep_and_load(
   db,
   source,
   table,
   res,
   do.reset = FALSE,
   do.insert = FALSE,
   chem.check.halt = FALSE
```

source_set_defaults 57

Arguments

db The version of toxval_source into which the source is loaded.

source Name of the source

table Name of the database table

res The data frame to be processed

do . reset If TRUE, delete data from the database for this source before inserting new data.

Default FALSE

chem.check.halt

If TRUE, stop the execution if there are errors in the chemical mapping

source_set_defaults

Set default value for NAs - jsut set NA to "-" for columns of type char-

acter

Description

Set default value for NAs - jsut set NA to "-" for columns of type character

Usage

```
source_set_defaults(res, source)
```

Arguments

res The input dataframe source The data source name

Value

Returns the input dataframe with defaults set

species.mapper Map the species to the ECOTOX species dictionary and export the missing species to add to the dictionary

Description

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

Usage

```
species.mapper(toxval.db, date_string = "2022-02-23")
```

Arguments

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

```
toxval.check.source_chemical
```

Check the status of the soruce_chemical tables

Description

Check the status of the soruce_chemical tables

Usage

```
toxval.check.source_chemical(toxval.db, source.db)
```

Arguments

toxval.db The version of toxvaldb to use.

source.db The vsource database version

toxval.config 59

toxval.config	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) and the urls for the ACToR web services.

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) and the urls for the ACToR web services.

Usage

```
toxval.config()
```

Value

Returns a set of parameters to be used throughout the package

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, reset = F)
```

Arguments

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

reset If TRUE, delete all content from the database

60 toxval.load.all

```
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

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=T) 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=T) 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,
  log = F,
  do.init = F,
  do.reset = F,
  do.load = F
```

toxval.load.atsdr 61

Arguments

toxval.db	The version of toxval into which the tables are loaded.
source.db	The version of toxvalsource database from which information is pulled.
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

toxval.load.atsdr Load the ATSDR MRLs 2020 data from toxval_source to toxval

Description

Load the ATSDR MRLs 2020 data from toxval_source to toxval

Usage

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

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.atsdr.pfas
```

Load the original ATSDR PFAS from toxval_source to toxval

Description

Load the original ATSDR PFAS from toxval_source to toxval

Usage

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

Arguments

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

source.db The source database to use.

62 toxval.load.bcfbaf

```
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 = F)
```

Arguments

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

source.db The source database to use.

log If TRUE, send messages to a log file

toxval.load.bcfbaf Load the Arnot BAF / BCF data

Description

Load the Arnot BAF / BCF data

Usage

```
toxval.load.bcfbaf(toxval.db, verbose = F)
```

Arguments

toxval.db The database to use.

verbose If TRUE, print out extra diagnostic messages

toxval.load.caloehha 63

```
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 = F)
```

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.cal_dph
```

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

Description

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

Usage

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

Arguments

toxval.db The database version to use

source.db The source database

64 toxval.load.chiu

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_201810-03.xlsx ../PPRTV_ORNL/PPRTV_ORNL cancer calls 2018-1025.xlsx ../cancer_summary/cancer/NTP/NTP cancer clean.xlsx ../can-

cer_summary/cancer/IARC/IARC cancer 2018-10-29.xlsx ../cancer_summary/cancer/HealthCanada/HealthCanada_TRVs_2010_AppendixA v2.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

Usage

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

Arguments

toxval.db The version of the database to use

toxval.load.chiu Load the Chiu data from toxval_source to toxval

Description

Load the Chiu data from toxval source to toxval

Usage

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

Arguments

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

source.db The source database to use.

toxval.load.copper 65

toxval.load.copper Load Copper Manufacturers daa from toxval_source to toxval

Description

Load Copper Manufacturers daa from toxval_source to toxval

Usage

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

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.cosmos Load teh COSMOS data from source to toxval

Description

Load teh COSMOS data from source to toxval

Usage

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

Arguments

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

source.db The source database to use.

66 toxval.load.dod.ered

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 = F)
```

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.dod.ered
```

Load the DOD ERED data from toxval_source to toxval

Description

Load the DOD ERED data from toxval source to toxval

Usage

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

Arguments

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

source.db The source database to use.

toxval.load.doe.benchmarks 67

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

Load DOE Wildlife Benchmarksdata from toxval_source to toxval

Description

Load DOE Wildlife Benchmarksdata from toxval_source to toxval

Usage

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

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.doe.ecorisk
```

Load the DOE ECORISK data (also called LANL) data from toxval_source to toxval

Description

Load the DOE ECORISK data (also called LANL) data from toxval_source to toxval

Usage

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

Arguments

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

 $\verb|source.db| \qquad \text{The version of toxval_source from which the tables are loaded}.$

```
toxval.load.doe.pac
```

Load DOE Protective Action Criteria data from toxval_source to toxval

Description

Load DOE Protective Action Criteria data from toxval_source to toxval

Usage

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

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.echa.echemportal.api
```

Load ECHA eChemPortal API data from toxval_source to toxval

Description

Load ECHA eChemPortal API data from toxval_source to toxval

Usage

```
toxval.load.echa.echemportal.api(toxval.db, source.db, log = F)
```

Arguments

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

source.db The source database to use.

toxval.load.ecotox 69

toxval.load.ecotox *Load ECOTOX from the web services output to toxval*

Description

Load ECOTOX from the web services output to toxval

Usage

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

Arguments

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

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 = F)
```

Arguments

 ${\tt toxval.db} \qquad {\tt The\ version\ of\ toxval\ into\ which\ the\ tables\ are\ loaded}.$

source.db The source database to use.

70 toxval.load.envirotox

toxval.load.efsa2 Load EFSA2 data from toxval_source to toxval

Description

Load EFSA2 data from toxval_source to toxval

Usage

```
toxval.load.efsa2(toxval.db, source.db, log = F)
```

Arguments

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

source.db The source databse from which data should be loaded

log If TRUE, send output to a log file

```
toxval.load.envirotox
```

Load EnviroTox data from toxval_source to toxval

Description

Load EnviroTox data from toxval source to toxval

Usage

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

Arguments

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

source.db The source database to use.

toxval.load.epa_aegl 71

```
toxval.load.epa_aegl
```

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

Description

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

Usage

```
toxval.load.epa_aegl(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.fda_cedi
```

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

Description

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

Usage

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

Arguments

toxval.db The database version to use

source.db The source database

72 toxval.load.genetox

```
toxval.load.generic
```

Generic structure for laoding to toxval from toxval_source

Description

Generic structure for laoding to toxval from toxval_source

Usage

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

Arguments

source.db The source database

log If TRUE, send output to a log file

toxval.db The database version to use

toxval.load.genetox

Load the Genetox data from Grace

Description

Load the Genetox data from Grace

Usage

```
toxval.load.genetox(toxval.db, verbose = F, do.read = T)
```

Arguments

toxval.db The database to use.

verbose If TRUE output debug information do.read If TRUE, read in the DSSTox file

```
toxval.load.genetox_details
```

Load the Genetox data from Grace

Description

Load the Genetox data from Grace

Usage

```
toxval.load.genetox_details(toxval.db, verbose = F)
```

Arguments

toxval.db The database to use.

verbose if TRUE output debug information

 ${\tt toxval.load.hawc} \quad \textit{Load HAWC from toxval_source to toxval}$

Description

Load HAWC from toxval_source to toxval

Usage

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

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.

```
toxval.load.hawc_pfas_150
```

Load HAWC PFAS 150 from toxval_source to toxval

Description

Load HAWC PFAS 150 from toxval_source to toxval

Usage

```
toxval.load.hawc_pfas_150(toxval.db, source.db, log = F)
```

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

```
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 = F)
```

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.

toxval.load.healthcanada 75

```
toxval.load.healthcanada
```

Load Health Canada data from toxval_source to toxval

Description

Load Health Canada data from toxval_source to toxval

Usage

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

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

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 = F)
```

Arguments

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

source.db The source database to use.

76 toxval.load.hpvis

toxval.load.hess Load the HESS data from toxval_source to toxval

Description

Load the HESS data from toxval_source to toxval

Usage

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

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.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 = F)
```

Arguments

toxval.db	The version of toxval into which the tables are loaded.
source.db	The source databse from which data should be loaded
loa	If TRUE, send output to a log file

toxval.load.iris 77

Description

Load new_iris_noncancer and new_iris_cancer from toxval_source to toxval

Usage

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

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.mass_mmcl

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

Description

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

Usage

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

Arguments

toxval.db The database version to use

source.db The source database

78 toxval.load.niosh

```
toxval.load.new_ecotox
```

Load ecotox data from datahub to toxval

Description

Load ecotox data from datahub to toxval

Usage

```
toxval.load.new_ecotox(toxval.db, verbose = T)
```

Arguments

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

verbose Whether the loaded rows should be printed to the console.

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 = F)
```

Arguments

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

source.db The source database to use.

toxval.load.opp 79

toxval.load.opp

Load opp from toxval_source to toxval

Description

Load opp from toxval_source to toxval

Usage

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

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

toxval.load.oppt Load new_oppt_table from toxval_source to toxval

Description

Load new_oppt_table from toxval_source to toxval

Usage

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

Arguments

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

source.db The source database to use.

80 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

```
toxval.load.ow_dwsha
```

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

Description

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

Usage

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

Arguments

toxval.db The database version to use

source.db The source database

toxval.load.penn 81

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 = F)
```

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.penn_dep
```

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

Description

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

Usage

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

Arguments

toxval.db The database version to use

source.db The source database

```
toxval.load.pfas_150_sem
```

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

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.pfas_summary_pods

Load PFAS Summary PODs from toxval_source to toxval

Description

Load PFAS Summary PODs from toxval_source to toxval

Usage

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

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.

toxval.load.postprocess 83

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 = F)
```

Arguments

toxval.db The database version to use

source The source name

do.convert.units

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

bugged

sourcedb The source database name

toxval.load.pprtv.ncea

Load PPRTV (NCEA) from toxval source to toxval

Description

Load PPRTV (NCEA) from toxval source to toxval

Usage

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

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.

84 toxval.load.rsl

```
toxval.load.pprtv.ornl
```

 $Load\ PPRTV\ (ORNL)\ from\ toxval_source\ to\ toxval$

Description

Load PPRTV (ORNL) from toxval_source to toxval

Usage

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

Arguments

toxval.db	The version of toxval into which the tables are loaded.
source.db	The source databse from which data should be loaded
log	If TRUE, send output to a log file

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 = F)
```

Arguments

toxval.db The database version to use

source.db The source database

toxval.load.skin.eye 85

```
toxval.load.skin.eye
```

Load the Skin eye data

Description

Load the Skin eye data

Usage

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

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 = T)
```

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
```

86 toxval.load.test

```
toxval.load.species
```

Load the species table and the species_id column in toxval

Description

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

Usage

```
toxval.load.species(toxval.db, restart = F, date_string = "2022-05-25")
```

Arguments

toxval.db The version of the database to use

restart If TRUE, rest all of the species_id values in toxval

date.string Date suffix on the input species dictionary

Description

Load TEST data from toxval source to toxval

Usage

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

Arguments

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

source.db The source database to use.

toxval.load.toxrefdb3 87

```
toxval.load.toxrefdb3
```

Load ToxRefdb data to toxval

Description

Load ToxRefdb data to toxval

Usage

```
toxval.load.toxrefdb3(toxval.db, source.db, log = F, do.init = F)
```

Arguments

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

log If TRUE, send output to a log file

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

verbose Whether the loaded rows should be printed to the console.

```
toxval.load.usgs_hbsl
```

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

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

88 toxval.load.wignall

```
toxval.load.who_ipcs
```

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

Description

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

Usage

```
toxval.load.who_ipcs(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.wignall
```

Load Wignall from toxval_source to toxval

Description

Load Wignall from toxval_source to toxval

Usage

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

Arguments

toxval.db	The version	of toxval	into which	the tables at	re loaded.

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

toxval.qc.step.1

```
{\it toxval.qc.step.1} \qquad {\it do~an~initial~QC~of~the~data~by~comparing~the~current~database~to~an} \\ {\it old~one}
```

Description

do an initial QC of the data by comparing the current database to an old one

Usage

```
toxval.qc.step.1(db.new = "res_toxval_v92", db.old = "dev_toxval_v9_1")
```

Arguments

db.new The new database version (toxval) for the comparison

db.old = The old database version for the comparison

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)
```

Arguments

toxval.db The database version to use

source The source

```
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.

```
toxval_source.hash.and.load
```

Add the hash key to the source tables and add the new rows

Description

Add the hash key to the source tables and add the new rows

Usage

```
toxval_source.hash.and.load(
  db = "dev_toxval_source_v5",
  source,
  table,
  do.reset = F,
  do.insert = F,
  res
)
```

Arguments

db	The version of toxval_source into which the source is loaded.
source	Name of the source
table	Name of the database table
do.reset	If TRUE, delete data from the database for this source before inserting new data. Default FALSE
do.insert	If TRUE, insert data into the database, default TRUE
res	The data frame to be processed

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