toxvaldb09

August 5, 2022

```
Type Package
Title Builds the ToxValDB V9.2 Database
Version 1.0.1
Author Aswani Unikrishnan
Maintainer Richard Judson < judson.richard@epa.gov>
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-
      ple sources
      into a single format. 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.
Imports DBI,
     RMySQL,
     openxlsx,
      dplyr,
      tidyr,
      stringr,
      tibble,
      janitor,
     XML,
      logr,
      miniUI,
      RCurl,
      gsubfn,
      textclean
License MIT + file LICENSE
Encoding UTF-8
LazyData true
RoxygenNote 7.2.1
Suggests knitr,
```

rmarkdown **VignetteBuilder** knitr

R topics documented:

build_echa_echemportal_api_dict	8
cas_checkSum	
chem.check	
chem.check.v2	
clean.last.character	
clean.toxval.by.source	
clowder_document_list	
clowder_id_prep.v3	
compare.pfas_150_sem.to.hawc	
contains	
echemportal.prep.v2	14
echemportal.prep.v2.step2	14
echemportal.prep.v2.step3	14
ecotox.datahub.to.file	15
efsa.clean	15
efsa.dict.prep	
efsa.prep	
export.all.by.source	
export.all.by.source.for.release	
export.all.by.source.pfas	
export.all.with.references	
export.bcfbaf	
export.cancer.summary	
•	
export.chemicals	
export.dsstox	
export.dsstox.mol.wt	
export.echa.repeats	
export.final.params	
export.genetox_details	
export.genetox_summary	
export.missing.rac	
export.missing.rac.by.source	
export.missing.strains	24
export.pod.summary	24
export.record_source	25
export.skin_eye	25
export.source_chemical	26
export.toxval_dictionary	26
fill.chemical	27
fill.chemical.by.source	27
fill.chemical_source_index	28
fill.toxval.defaults	28
fill.toxval.defaults.global	29
fill.toxval.defaults.global.by.source	29
fix.all.param	30
fix.all.param.by.source	30

fix.all.param.new						
fix.all.param.new.by.source						
fix.casrn						
fix.clowder_id.by.source						
fix.clowder_id.by.toxval	 	 	 	 		. 33
fix.critical_effect	 	 	 	 		. 33
fix.critical_effect.icf.by.source	 	 	 	 		. 34
fix.empty	 	 	 	 		. 34
fix.empty.by.source	 	 	 	 		. 35
fix.empty.hyphen.record_source.by.source	 	 	 	 		. 35
fix.empty.record_source	 	 	 	 		. 36
fix.empty.record_source.by.source	 	 	 	 		. 36
fix.exposure_form						
fix.exposure_form.by.source						
fix.exposure_method.and.form.by.source .						
fix.exposure_route.by.type						
fix.exposure_route.by.type.new						
fix.exposure_route.by.type.new.by.source						
fix.generation.by.source						
fix.human_eco						
fix.human_eco.by.source						
fix.hyphen.by.source						
fix.non_ascii						
fix.non_ascii.v2						
fix.priority_id						
fix.priority_id.by.source						
fix.qa_status	 	 	 	 • •		. 43 . 44
fix.qa_status.by.source						
fix.qc_status.by.source	 	 	 	 • •	• •	. 44
fix.risk_assessment_class						
fix.risk_assessment_class.all.source						
fix.risk_assessment_class.by.source						
fix.single.param						
fix.single.param.by.source	 	 	 	 		. 47
fix.single.param.new	 	 	 	 		. 47
fix.single.param.new.by.source	 	 	 	 		. 48
fix.species						
fix.species.by.source	 	 	 	 		. 49
fix.species.ecotox.by.source						
fix.species.v2						
fix.species_ecotox	 	 	 	 		. 50
fix.strain.by.source	 	 	 	 		. 51
fix.strain.v2						
fix.toxval_numeric_qualifier	 	 	 	 		. 52
fix.toxval_numeric_qualifier.by.source	 	 	 	 		. 52
fix.units	 	 	 	 		. 53
fix.units.by.source						. 53
fix units new						54

fix.units.new.by.source	 :	55
fix.units.testmw	 :	56
format_rsl_excel	 	56
generate.originals		57
get.chemical.info.by.source	 	57
get.chemical.info.by.source.combined		58
get.cid.list.toxval		58
get.cid.list.toxval.ecotox		59
get.clowder.file.maps		59
getDBConn		60
getPSQLDBConn		60
get_clowder_docList		61
heast.load.all	 	61
hess_record_url_from_clowder		62
ig.summary.plot		62
import.dictionary		63
import.driver		63
1		64
import.source.info		04 64
import.source.info.by.source		
import_actor_source		65
import_atsdr_pfas_2021_source		65
import_atsdr_pfas_source		66
import_atsdr_source		66
import_caloehha_source		67
import_chiu_source		67
import_copper_source		68
import_cosmos_source		69
import_dod_ered_source		69
import_dod_source		7 0
import_doe_benchmarks_source	 ′	7 0
import_doe_source	 ′	71
import_echa3_source		71
import_echa_echemportal_api_source		72
import_echa_echemportal_source		73
import_echa_iuclid_source		73
import_echa_source		74
import_efsa2_source		74
import_efsa_source		75
import envirotox source		75
import_flex_source		76
import_generic_source		77
import_hawc_pfas_150_source		, , 77
import_hawc_pfas_430_source		, , 78
		79
import_hawc_source		19 79
import_health_canada_source		
import_heast_source		80
import_hess_source		80
import hpvis source	 	81

import_iris_source	81
import_lanl_source	82
import_niosh_source	82
import_oppt_source	83
import_opp_source	83
import_penn_source	84
import_pfas_150_sem_v2_source	84
import_pprtv_ncea_source	85
import_pprtv_ornl_source	85
import_rsl_source	86
import_rsl_source_info	87
import_test_source	87
import_wignall_source	88
iris.cancer.clean	88
iris.noncancer.clean	89
iris.scraper	89
load.dsstox	89
load_clowder_document_name	90
log_message	90
map.chemical.to.dsstox	91
map.chemical.to.dsstox.by.source	91
map.chemical.to.dsstox.ecotox	92
map.chemical_list.to.dsstox	92
map.hash.record.clowder.document_name	93
map.hash.record_source	93
map.hash.record_source.by.source	94
niosh.pdf.to.excel	94
parse.effect.level	95
•	95
pfas.by.source	96
pprtv.ncea.load.all	96
	97
pprtv.ncea.scraper	97
pprtv.ornl.load.all.new	97
pprtv.ornl.scraper	98
printCurrentFunction	
reset.numeric	98
runInsert	99
runInsertTable	99
runQuery	
runQuery_psql	
runStatement	
set.dtxsid	
set.dtxsid.by.source	
set.hash.bcfbaf	
set.hash.bcfbaf.by.source	
set.hash.genetox_details	
set.hash.genetox_details.by.source	
set.hash.record_source	104

set.hash.record_source.by.source	
set.hash.skin_eye	
set.hash.skin_eye.by.source	
set.hash.source	106
set.hash.toxval	107
set.hash.toxval.by.source	107
setDBConn	108
setPSQLDBConn	108
set_clowder_id	109
source.size	
source.table.to.DAT	
source_chemical.duplicates	
source_chemical.ecotox	
source_chemical.process	
source_chemical.toxrefdb	
source_prep_and_load	
source_set_defaults	
species.mapper	
toxval.check.source_chemical	
toxval.config	
toxval.init.db	
toxval.load.alaska_dec	
toxval.load.all	
toxval.load.atsdr	
toxval.load.atsdr.pfas	
toxval.load.atsdr.pfas.2021	
toxval.load.bcfbaf	
toxval.load.caloehha	
toxval.load.cal_dph	
toxval.load.cancer	
toxval.load.chemical.list	
toxval.load.chemical.list.by.source	
toxval.load.chemical.list.ecotox	
toxval.load.chiu	
toxval.load.copper	
toxval.load.cosmos	
toxval.load.dod	
toxval.load.dod.ered	
toxval.load.doe	
toxval.load.doe.benchmarks	
toxval.load.doe.ecorisk	
toxval.load.doe.pac	
toxval.load.echa.echemportal.api	
toxval.load.ecotox	
toxval.load.efsa	
toxval.load.efsa2	
toxval.load.envirotox	
toxval.load.epa aegl	130

Index

152

toxval.load.fda_cedi
toxval.load.flex
toxval.load.generic
toxval.load.genetox
toxval.load.genetox_details
toxval.load.hawc
toxval.load.hawc_pfas_150
toxval.load.hawc_pfas_430
toxval.load.healthcanada
toxval.load.heast
toxval.load.hess
toxval.load.hpvis
toxval.load.initial
toxval.load.iris
toxval.load.mass_mmcl
toxval.load.new_ecotox
toxval.load.niosh
toxval.load.opp
toxval.load.oppt
toxval.load.osha_air_limits
toxval.load.ow_dwsha
toxval.load.penn
toxval.load.penn_dep
toxval.load.pfas_150_sem_v2
toxval.load.postprocess
toxval.load.pprtv.ncea
toxval.load.pprtv.ornl
toxval.load.rsl
toxval.load.skin.eye
toxval.load.source_chemical
toxval.load.species
toxval.load.test
toxval.load.toxrefdb3
toxval.load.usgs_hbsl
toxval.load.who_ipcs
toxval.load.wignall
toxval.qc.step.1
toxval.set.mw
toxval.source.add.timestamps
toxval.source.map.chemicals
toxval.source.map.chemicals.combined
toxval.summary.stats
toxval_source.hash.and.load

8 cas_checkSum

Description

code to create ECHA echemportal api dict

Usage

```
build_echa_echemportal_api_dict(toxval.db, filepath)
```

Arguments

toxval.db	The version of toxval into which the dictionary is loaded.
filepath	The path for all the input xlsx files ./echa_echemportal_api/echa_echemportal_api_files

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

x 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 <code>cas_detect</code> function to check CAS format beforehand, or write your own function if necessary.

chem.check 9

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))
```

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

Usage

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

10 chem.check.v2

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=c

clean.last.character 11

```
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

12 clowder_id_prep.v3

```
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

```
compare.pfas_150_sem.to.hawc
```

Compare teh PFAS 150 SEM and hte corresponding HAWC data

Description

Compare teh PFAS 150 SEM and hte corresponding HAWC data

Usage

```
compare.pfas_150_sem.to.hawc(db)
```

Arguments

db

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

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

```
echemportal.prep.v2
```

Process the ECHA eChemPortal data from 2020

Description

Process the ECHA eChemPortal data from 2020

Usage

```
echemportal.prep.v2(do.load = F)
```

Arguments

do.load

If TRUE, laod all of the in vivo data

```
echemportal.prep.v2.step2
```

Process the ECHA eChemPortal data from 2020 - step 2

Description

Process the ECHA eChemPortal data from 2020 - step 2

Usage

```
echemportal.prep.v2.step2(do.load = F)
```

Arguments

do.load

If TRUE, laod all of the in vivo data

```
echemportal.prep.v2.step3
```

Process the ECHA eChemPortal data from 2020 - step 3

Description

Process the ECHA eChemPortal data from 2020 - step 3

Usage

```
echemportal.prep.v2.step3(do.load = F)
```

Arguments

do.load

If TRUE, laod all of the in vivo data

ecotox.datahub.to.file

```
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

toxval.db	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

efsa.clean prepare EFSA_combined.xlsx using dictionaries from efsa.dict.prep.R to be loaded into dev_toxval_source_v4.

Description

prepare EFSA_combined.xlsx using dictionaries from efsa.dict.prep.R to be loaded into dev_toxval_source_v4.

Usage

```
efsa.clean(dir, verbose = F)
```

Arguments

dir The directory where the input data sits, ../efsa2/efsa2_files/

16 efsa.prep

${\it efsa.dict.prep} \qquad {\it Create dictionaries for preparing EFSA_combined.xlsx\ produced\ from efsa.prep.R}$	n
---	---

Description

Create dictionaries for preparing EFSA_combined.xlsx produced from efsa.prep.R

Usage

```
efsa.dict.prep(dir)
```

Arguments

dir The directory where the input data sits, ../efsa2/efsa2_files/

efsa.prep	Prepare the new EFSA data	

Description

Prepare the new EFSA data

Usage

```
efsa.prep(dir, step1 = F, step2 = F, step3 = F, step4 = F)
```

Arguments

dir	The directory where the input data sits,/efsa2/efsa2_files/
step1	Run the first step of the processing
step2	Run the second step of the processing
step3	Run the third step of the processing
step4	Run the fourth step of the processing

export.all.by.source 17

```
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

toxval.db Database version

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.by.source.for.release
```

Build a data frame of the data from toxval and export by source as a series of xlsx files. This only has the columns the someone outside might use

Description

Build a data frame of the data from toxval and export by source as a series of xlsx files. This only has the columns tht someone outside might use

Usage

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

Arguments

t 111-	Databasassasias	_
toxval.db	Database version	n

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.by.source.pfas
```

Build a data frame of the data from toxval and export by source as a series of xlsx files. This is a version for PFAS specific use

Description

Build a data frame of the data from toxval and export by source as a series of xlsx files. THis is a version for PFAS specific use

Usage

```
export.all.by.source.pfas(toxval.db)
```

Arguments

toxval.db Database version
source The source to be updated

Value

Write a file with the results

```
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 Build a data frame of the PODs and exports as xlsx

Usage

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

Arguments

toxval.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'

export.bcfbaf 19

Value

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

export.bcfbaf

Export the BCF / BAF data data

Description

Export the BCF / BAF data data

Usage

```
export.bcfbaf(toxval.db, dir = "./export")
```

Arguments

toxval.db Database version

Value

writes and Excel file with the name ../qc_export/toxval_genetox_details_[Sys.Date].xlsx

```
export.cancer.summary
```

Build a data frame of the Cancer calls and exports as xlsx

Description

Build a data frame of the Cancer calls and exports as xlsx

Usage

```
export.cancer.summary(toxval.db, file.name = NA, dir = "./export")
```

Arguments

toxval.db Database version

file.name If not NULL, read afles of casrn from the chemical folder and only export those

chemicals

Value

writes and Excel file with the name ../qc_export/toxval_pod_summary_min_quality_id_[human_eco]_[min_quality_id]_[Sys

20 export.dsstox.mol.wt

export.chemicals

Export all chemicals in the chemical and chemical_list tables

Description

Export all chemicals in the chemical and chemical_list tables

Usage

```
export.chemicals(toxval.db)
```

Arguments

```
toxval.db Database version
```

Value

writes and Excel file with the name ../export/toxval_chemicals_[Sys.Date].xlsx

export.dsstox

Export the DSSTox chemical table

Description

Export the DSSTox chemical table

Usage

```
export.dsstox()
```

```
export.dsstox.mol.wt
```

Export mol weight from DSSTox

Description

Export mol weight from DSSTox

Usage

```
export.dsstox.mol.wt()
```

export.echa.repeats 21

```
export.echa.repeats
```

Export ECHA data from all four ECHA sources and look for overlaps

Description

Export ECHA data from all four ECHA sources and look for overlaps

Usage

```
export.echa.repeats(toxval.db)
```

Arguments

```
toxval.db Database version
```

Value

writes and Excel file with the name ./export/toxval_echa_repeats_[Sys.Date].xlsx

```
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.genetox_details
```

Export the detailed genetox data

Description

Export the detailed genetox data

Usage

```
export.genetox_details(toxval.db, dir = "./export")
```

Arguments

toxval.db Database version

Value

writes and Excel file with the name ../qc_export/toxval_genetox_details_[Sys.Date].xlsx

```
export.genetox_summary
```

Export the summary genetox data

Description

Export the summary genetox data

Usage

```
export.genetox_summary(toxval.db, dir = "./export")
```

Arguments

toxval.db Database version

Value

writes and Excel file with the name ../qc_export/toxval_genetox_summary_[Sys.Date].xlsx

export.missing.rac 23

export.missing.rac Export the rows with a missing risk_assessment_class

Description

Export the rows with a missing risk_assessment_class

Usage

```
export.missing.rac(toxval.db)
```

Arguments

```
toxval.db Database version
```

Value

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

```
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"

24 export.pod.summary

```
export.missing.strains
```

Set the strain information in toxval

Description

Set the strain information in toxval

Usage

```
export.missing.strains(toxval.db, date_string = "2022-05-25")
```

Arguments

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

export.pod.summary 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.pod.summary(
  toxval.db,
  human_eco = "human health",
  file.name = NA,
  dir = "./export"
)
```

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.record_source 25

```
export.record_source
```

Build a data frame of the th data from record_source and export

Description

Build a data frame of the th data from record_source and export

Usage

```
export.record_source(toxval.db, dir = "./export")
```

Arguments

```
toxval.db Database version
```

Value

writes an Excel file with the name ../export/toxval_record_summary_[Sys.Date].xlsx

```
export.skin_eye
```

Export the skin and eye data

Description

Export the skin and eye data

Usage

```
export.skin_eye(toxval.db, dir = "./export")
```

Arguments

```
toxval.db Database version
```

Value

writes and Excel file with the name ../qc_export/toxval_skin_eye_[Sys.Date].xlsx

```
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

```
export.toxval_dictionary
```

Export the toxval_dictionary table

Description

Export the toxval_dictionary table

Usage

```
export.toxval_dictionary(toxval.db, dir = "./export")
```

Arguments

```
toxval.db Database version
```

Value

writes and Excel file with the name ../qc_export/toxval_dictionary_[Sys.Date].xlsx

fill.chemical 27

fill.chemical

Fill the chemical table

Description

Fill the chemical table

Usage

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

Arguments

toxval.db The version of toxvaldb to use.

verbose If TRUE, print out extra diagnostic messages

```
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

28 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 Set Toxval Defaults globally
```

Description

Set Toxval Defaults globally

Usage

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

Arguments

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

```
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

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, generation

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, generation

Usage

```
fix.all.param(toxval.db)
```

Arguments

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

Value

The database will be altered

```
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

fix.all.param.new 31

Value

The database will be altered

fix.all.param.new 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, generation

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, generation

Usage

```
fix.all.param.new(toxval.db)
```

Arguments

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

Value

The database will be altered

```
fix.all.param.new.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.new.by.source(toxval.db, source)
```

Arguments

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

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.clowder_id.by.source
```

Add clowder_id's to source db tables based on matching values with source table

Description

Add clowder_id's to source db tables based on matching values with source table

Usage

```
fix.clowder_id.by.source(source.db, source_table, source)
```

Arguments

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

Value

```
fix.clowder_id.by.toxval
```

Add clowder_id's to source db tables

Description

Add clowder_id's to source db tables

Usage

```
fix.clowder_id.by.toxval(toxval.db, source.db, source_table, source, infile)
```

Arguments

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

infile The input file ./clowder_id_mapping/source_doc_with_clowder_id.xlsx, new_qa_set_with_ClowderID_1

22.csv,clowderid_record_source_hash_hawc_pfas_150_430_with_source_hash.xlsx,

atsdr_toxval_record_source_w_document-Aswani.csv,efsa2_toxval_record_source_w_document-Aswani.csv, original_oppt_table_w_document-Aswani.csv, subset_v8_chiu_record_source_hash-

Aswani.csv,WHOIPCS_v8_v9_should_be_same_record_source_hash-Aswani.csv,missing_toxval_source_hash-Aswani.csv

toxval_new_qa_set_ClowderID_02-02-ASWANI.csv, del_docs_matched_20220323.xlsx,

toxval_qa_set_2_ECHA-IUCLID_ClowderID_03-23_Aswani.csv

Value

The database will be altered

```
fix.critical_effect
```

Fix critical_effect in toxval table Fix occurances of multiple critical_effect in the toxval_critical_effect table based on values from critical_effect dictionary file

Description

Fix critical_effect in toxval table Fix occurances of multiple critical_effect in the toxval_critical_effect table based on values from critical_effect dictionary file

Usage

```
fix.critical_effect(toxval.db)
```

Arguments

toxval.db The version of toxvaldb to use.

fix.empty

```
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

Set all empty cells in toxval to '-'

Description

Set all empty cells in toxval to '-'

Usage

```
fix.empty(toxval.db)
```

Arguments

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

Value

fix.empty.by.source 35

```
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 'Not Specified'

Usage

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

Arguments

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

Value

```
fix.empty.record_source
```

Set all empty cells in record_source to '-'

Description

Set all empty cells in record_source to '-'

Usage

```
fix.empty.record_source(toxval.db)
```

Arguments

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

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

fix.exposure_form 37

Description

Exposure Method temporary fix to add Exposure Form

Usage

```
fix.exposure_form(toxval.db)
```

Arguments

toxval.db The database version to use

fix.exposure_form.by.source

Exposure Method temporary fix to add Exposure Form

Description

Exposure Method temporary fix to add Exposure Form

Usage

```
fix.exposure_form.by.source(toxval.db, source)
```

Arguments

toxval.db The database version to use

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.exposure_route.by.type
```

Alter the exposure route of toxval according to an excel dictionary

Description

Alter the exposure route of toxval according to an excel dictionary

Usage

```
fix.exposure_route.by.type(toxval.db)
```

Arguments

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

Value

The database will be altered

```
fix.exposure_route.by.type.new
```

Alter the exposure route of toxval according to an excel dictionary

Description

Alter the exposure route of toxval according to an excel dictionary

Usage

```
fix.exposure_route.by.type.new(toxval.db)
```

Arguments

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

Value

```
fix.exposure_route.by.type.new.by.source
```

Alter the exposure route and study_duration_class of toxval based on toxval_type

Description

Alter the exposure route and study_duration_class of toxval based on toxval_type

Usage

```
fix.exposure_route.by.type.new.by.source(toxval.db, source)
```

Arguments

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

Value

The database will be altered

```
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

fix.human_eco

Fix the human_eco flag

Description

Fix the human_eco flag

Usage

```
fix.human_eco(toxval.db, reset = T)
```

Arguments

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

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, reset = T)
```

Arguments

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

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

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

source

Value

fix.hyphen.by.source 41

```
fix.hyphen.by.source
```

Set all hyphen cells in toxval to 'Not Specified'

Description

Set all hyphen cells in toxval to 'Not Specified'

Usage

```
fix.hyphen.by.source(toxval.db, source)
```

Arguments

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

Value

The database will be altered

fix.non_ascii

Flag non ascii characters in the database

Description

Flag non ascii characters in the database

Usage

```
fix.non_ascii(df)
```

Value

The dataframe with non ascii characters replaced with XXX

fix.priority_id

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 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(toxval.db)
```

Arguments

toxval.db The version of toxvaldb to use.

```
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.qa_status

Fix the qa_status flag

Description

Fix the qa_status flag

Usage

```
fix.qa_status(toxval.db, reset = T)
```

Arguments

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

Value

Description

Fix the qa_status flag

Usage

```
fix.qa_status.by.source(toxval.db, source, reset = T)
```

Arguments

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

Value

The database will be altered

```
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

```
fix.risk_assessment_class
```

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(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.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

46 fix.single.param

```
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.single.param 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(toxval.db, param, ignore = FALSE)
```

Arguments

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

param THe parameter value to be fixed

ignore If TRUE allow missing values to be ignored

Value

```
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.single.param.new
```

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.new(toxval.db, param, ignore = FALSE)
```

Arguments

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

param THe parameter value to be fixed

ignore If TRUE allow missing values to be ignored

Value

fix.species

```
fix.single.param.new.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.new.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

ignore If TRUE allow missing values to be ignored

Value

The database will be altered

fix.species	Update the species information. This method has to be run iteratively
	to find the remaining species_original names that don't match what is

in the database

Description

Update the species information. This method has to be run iteratively to find the remaining species_original names that don't match what is in the database

Usage

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

Arguments

toxval.db The version of the database to use

fix.species.by.source 49

```
fix.species.by.source
```

Update the species information. This method has to be run iteratively to find the remaining species_original names that don't match what is in the database

Description

Update the species information. This method has to be run iteratively to find the remaining species_original names that don't match what is in the database

Usage

```
fix.species.by.source(toxval.db, source)
```

Arguments

toxval.db The version of the database to use

```
fix.species.ecotox.by.source
```

Update the species_id in toxval from species_ecotox.

Description

Update the species_id in toxval from species_ecotox.

Usage

```
fix.species.ecotox.by.source(toxval.db, source)
```

Arguments

toxval.db The version of the database to use

fix.species_ecotox

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.species_ecotox *Update the species ecotox table with habitat information from ecotox dictionary.*

Description

Update the species ecotox table with habitat information from ecotox dictionary.

Usage

```
fix.species_ecotox(toxval.db)
```

Arguments

toxval.db The version of the database to use

fix.strain.by.source 51

```
fix.strain.by.source
```

Update the strain_group in toxval from strain_dictionary_2022-03-07.xlsx.

Description

Update the strain_group in toxval from strain_dictionary_2022-03-07.xlsx.

Usage

```
fix.strain.by.source(toxval.db, source)
```

Arguments

toxval.db The version of the database to use

fix.strain.v2

Set the strain information in toxval

Description

Set the strain information in toxval

Usage

```
fix.strain.v2(toxval.db, source = NULL, date_string = "2022-08-04")
```

Arguments

toxval.db The version of the database to use

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

date_string The date of the latest dictionary version

Description

Fix the toxval_numeric_qualifier

Usage

```
fix.toxval_numeric_qualifier(toxval.db)
```

Arguments

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

Value

The database will be altered

Description

Fix the toxval_numeric_qualifier by source

Usage

```
fix.toxval_numeric_qualifier.by.source(toxval.db, source)
```

Arguments

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

Value

fix.units 53

fix.units

Do all of the fixes to units

Description

- 1. All of these steps operate on the toxval_units column.
- 2. To allow this to be run multiple times during debugging, the first step is to copy toxval_units_original into toxval_units
- 3. Replace variant unit names with standard ones, running fix.single.param. This fixes issues like variant names for mg/kg-day and uses the dictionary file dictionary/toxval_units_5.xlsx
- 4. Fix special characters in toxval_units
- 5. Fix issues with units containing extra characters for some ECOTOX records
- 6. 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
- 7. Run conversions from molar to mg units, using MW. This uses the dictionary file dictionary/MW conversions.xlsx
- 8. 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
- 9. 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
- 10. Make sure that eco studies are in mg/L and human health in mg/m3

Usage

```
fix.units(toxval.db, do.convert = T)
```

Arguments

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

do.convert If TRUE, so unit conversions, as opposed to just cleaning
```

```
fix.units.by.source
```

Do all of the fixes to units

54 fix.units.new

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)
```

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

fix.units.new

Do all of the fixes to units

Description

- 1. All of these steps operate on the toxval_units column.
- 2. To allow this to be run multiple times during debugging, the first step is to copy toxval_units_original into toxval_units
- 3. Replace variant unit names with standard ones, running fix.single.param. This fixes issues like variant names for mg/kg-day and uses the dictionary file dictionary/toxval_units_5.xlsx
- 4. Fix special characters in toxval_units
- 5. Fix issues with units containing extra characters for some ECOTOX records
- 6. 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

fix.units.new.by.source 55

7. Run conversions from molar to mg units, using MW. This uses the dictionary file dictionary/MW conversions.xlsx

- 8. 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
- 9. 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
- 10. Make sure that eco studies are in mg/L and human health in mg/m3

Usage

```
fix.units.new(toxval.db, do.convert = T)
```

Arguments

toxval.db The version of toxvaldb to use.

do.convert If TRUE, so unit conversions, as opposed to just cleaning

fix.units.new.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

56 format_rsl_excel

Usage

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

Arguments

toxval.db The version of toxvaldb to use.

do.convert If TRUE, so unit conversions, as opposed to just cleaning

fix.units.testmw Do all of the fixes to units

Description

Do all of the fixes to units

Usage

```
fix.units.testmw(toxval.db = "dev_toxval_v9", do.convert = T)
```

Arguments

toxval.db The version of toxvaldb to use.

do.convert If TRUE, so unit conversions, as opposed to just cleaning

format_rsl_excel Convert complex rsl Source xlsx files into formatted rsl xlsx source files.

Description

Convert complex rsl Source xlsx files into formatted rsl xlsx source files.

Usage

```
format_rsl_excel(x, thq_x, y, thq_y, z)
```

Arguments

Х	./rsl/rsl_files/rsl_thq1_nov_2021.xlsx - The downloaded xls summary table for THQ 1 from RSL-Generic Tables (2020)
thq_x	corresponding thq for x, which is 1 here.
thq <u>y</u>	corresponding thq for y, which is 0.1 here.
Y	./rsl/rsl_files/rsl_thq0.1_nov_2021.xlsx - The downloaded xls summary table for THQ 0.1 from RSL-Generic Tables (2020)
Z	$./rsl/rsl_files/rsl_subchronic_nov_2021.xlsx-\ downloaded\ subchronic\ toxicity\ table$

generate.originals 57

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

Description

get chemical info from source db tables

Usage

```
get.chemical.info.by.source(source.db, source_table, source, file_id)
```

Arguments

source_table The name of toxval source to use.

source The name of toxval source table to use.

file_id The suffixed 5 digit identifiers specified in the file names in the folder ./chemical_mapping/source_chemical_files

Value

database info collected

58 get.cid.list.toxval

Description

get chemical info from source db tables for curation, create chemical table to map curated chemicals to.

Usage

```
get.chemical.info.by.source.combined(source.db, source_table, source)
```

Arguments

```
source_table The name of toxval source to use.

Source The name of toxval source to use.

The name of toxval source to use.
```

Value

database info collected

```
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

Value

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

get.cid.list.toxval.ecotox 59

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

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.ecotox(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

Value

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

Description

Pull Clowder file information to map to toxval records

Usage

```
get.clowder.file.maps(apiKey)
```

Arguments

apiKey

User Clowder API key to access Clowder

Value

Dataframe list of Clowder ID maps

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

```
getDBConn()
```

Value

print the database connection information

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

get_clowder_docList 61

```
get_clowder_docList
```

Get Clowder Document List

Description

This is a helper function to get a list of documents available in a Clowder dataset

Usage

```
get_clowder_docList(apiKey, clowder_dataset)
```

Arguments

```
apiKey The API key required for a user to access the Clowder dataset clowder_dataset
```

A character string for the dataset name

Value

Returns a dataframe with file details of: file size, date_created, file type, file id, and filename

```
heast.load.all Load HEAST to toxval_source. The data to be loaded is in the file ./heast/heast_files/EPA_HEAST_Table1_ORNL for loading.xlsx
```

Description

Load HEAST to toxval_source. The data to be loaded is in the file ./heast/heast_files/EPA_HEAST_Table1_ORNL for loading.xlsx

Usage

```
heast.load.all(source.db)
```

Arguments

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

62 ig.summary.plot

```
hess_record_url_from_clowder
```

Get record urls for hess documents from clowder

Description

Get record urls for hess documents from clowder

Usage

```
hess_record_url_from_clowder(toxval.db, source.db, apiKey, clowder_dataset)
```

Arguments

toxval.db	The version of toxval in which the data is altered.
source.db	The version of toxval source into which clowder data is loaded.
apiKey	The API key required for a user to access the Clowder dataset, prefix the apiKey value with "?key="
clowder_datas	set
	A character string for the dataset name apiKey="", clowder_dataset="CCTE

A character string for the dataset name apiKey="", clowder_dataset="CCTE ToxValDB PDFs"

```
ig.summary.plot
```

Make a plot summarizing the IG flag information

Description

Make a plot summarizing the IG flag information

Usage

```
ig.summary.plot(to.file = F, sys.date, do.read = F)
```

Arguments

to.file	If TRUE, print the graph to a file, else write to the screen
sys.date	The date of the bin data Excel fileto read
do.read	if TRUE, read in the source file and store in a global

import.dictionary 63

import.dictionary import the toxval and toxval_type dictionaries

Description

import the toxval and toxval_type dictionaries import the toxval and toxval_type dictionaries by source

Usage

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

Arguments

toxval.db The name of the database

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_actor_source 65

```
import_actor_source
```

Extract ACToR1 data to toxval source

Description

Extract ACToR1 data to toxval source

Usage

```
import_actor_source(toxval.db, infile, filepath, verbose = F)
```

Arguments

toxval.db	The version of toxval source into which the tables are loaded.
infile	The input file ./ACToR replacements/ACToR_2021/assay_table_hazard prioritized for use.xlsx
filepath	The path for all the input xlsx files ./ACToR replacements/ACToR_2021
verbose	Whether the loaded rows should be printed to the console.
do.init	if TRUE, read the data in from the res_actor_2021q4 database and set up the matrix

```
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
```

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 69

```
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.

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

 $infile 2 \qquad The input file ./cosmos/cosmos_files/COSMOS_DB_v1_export_2016_04_02_cosmetics_inventory.xlsx$

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

 ${\tt db}$ ${\tt The\ version\ of\ toxval_source}$ into which the tables are loaded. chem.check.halt

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 71

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

Description

Load DOE Source into toxval_source Load doe Source into dev_toxval_source_v4.

Usage

```
import_doe_source(toxval.db, infile)
import_doe_source(toxval.db, infile)
```

Arguments

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

infile The input file ./doe/doe_files/Revision_29.xlsx

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_echa3_source
```

Load ECHA TSCA POC Source into dev_toxval_source_v4.

Description

Load ECHA TSCA POC Source into dev_toxval_source_v4.

Usage

```
import_echa3_source(
  toxval.db,
  infile,
  dict_toxval_units,
  dict_toxval_type,
  dict_study_type,
  dict_exposure_route,
  dict_exposure_method,
  dict_study_duration,
  dict_species,
  dict_critical_effects)
```

Arguments

```
toxval.db
                 The version of toxval into which the source is loaded.
infile
                 The input file ./echa3/echa3_files/TSCA_POC_Chemical_Results_081220.xlsx
dict_toxval_units
                 The input file ./echa3/echa3_files/toxval_units_dictionary.xlsx
dict_toxval_type
                 The input file ./echa3/echa3_files/toxval_type_dictionary.xlsx
dict_study_type
                 The input file ./echa3/echa3_files/study_type_dictionary.xlsx
dict_exposure_route
                 The input file ./echa3/echa3_files/exposure_route_dictionary.xlsx
dict_exposure_method
                 The input file ./echa3/echa3_files/exposure_method_dictionary.xlsx
dict_study_duration
                 The input file ./echa3/echa3_files/study_duration_dictionary.xlsx
dict_species The input file ./echa3/echa3_files/echa3_species_dict.xlsx
dict critical effects
                 The input file ./echa3/echa3_files/critical_effect_dictionary.xlsx
```

```
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.

filepath The path for all the input xlsx files ./echa_echemportal_api/echa_echemportal_api_files chem.check.halt

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

```
import_echa_echemportal_source
```

Load ECHA echemportal 2020 Source into dev_toxval_source_v4.

Description

Load ECHA echemportal 2020 Source into dev_toxval_source_v4.

Usage

```
import_echa_echemportal_source(toxval.db, infile)
```

Arguments

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

 $\verb|infile| In the input file ./echa_echemportal/echa_echemportal_files/eChemPortal mam-principle and the input file ./echa_echemportal_files/eChemPortal mam-principle and ./echa_echemportal_files/eChemPortal mam-principle and ./echa_echemportal_files/eChemPortal mam-principle and ./echa_echemportal_files/eChemPorta$

malian data 2020 step 3.xlsx ,build from echemportal.prep.v2.step3.R

```
import_echa_iuclid_source
```

Load ECHA IUCLID Source into dev_toxval_source_v4.

Description

Load ECHA IUCLID Source into dev_toxval_source_v4.

Usage

```
import_echa_iuclid_source(toxval.db, infile, verbose = T)
```

Arguments

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

infile The input file ./echa_iuclid/echa_iuclid_files/echa_iuclid_v8.xlsx

74 import_efsa2_source

Description

Load ECHA Source from dev_toxval_source_v4(used in v8) saved as infile to dev_toxval_source_v4

Usage

```
import_echa_source(toxval.db, infile, verbose = T)
```

Arguments

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

infile The input file /echa/echa_files/echa_raw.xlsx
```

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
```

75 import_efsa_source

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

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

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

import_envirotox_source

Load EnviroTox.V2 Source data into dev_toxval_source_v4.

Description

Load EnviroTox.V2 Source data into dev_toxval_source_v4.

Load EnviroTox.V2 Source data into toxval_source

76 import_flex_source

Usage

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

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

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

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.

import_generic_source 77

```
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

```
import_generic_source
```

A generic tmpalte for adding data to toxval_source for a new source

Description

A generic tmpalte for adding data to toxval_source for a new source

Usage

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

Arguments

 $\begin{tabular}{ll} \begin{tabular}{ll} \beg$

If TRUE and there are bad chemical names or casrn,

Description

Load HAWC PFAS 150 Source into toxval_source

```
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

```
import_hawc_pfas_430_source
```

Load HAWC PFAS 430 Source into toxval_source

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 79

```
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

Description

Load Health Canada Source Info into toxval_source

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

80 import_hess_source

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
```

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

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

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

infile The input file ./heast/heast_files/EPA_HEAST_Table1_ORNL for loading.xlsx chem.check.halt
```

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

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

import_hpvis_source 81

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

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

```
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

```
\verb|import_iris_source| \textit{Load IRIS Source into toxval\_source}|
```

Description

Load IRIS Source into toxval_source

```
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
)
```

82 import_niosh_source

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

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

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

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

import_oppt_source 83

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

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

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_v2_source
```

Load PFAS 150 SEM V2 Source data into toxval_source

Description

Load PFAS 150 SEM V2 Source data into toxval_source

Usage

```
import_pfas_150_sem_v2_source(db, chem.check.halt = F)
```

Arguments

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

```
import_pprtv_ornl_source
```

Load PPRTV ORNL Source into toxval_source

Description

Load PPRTV ORNL Source into toxval_source

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

86 import_rsl_source

Arguments

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

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

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

Description

Load rsl Source Info into dev_toxval_source_v2.

Usage

```
import_rsl_source_info(toxval.db, infile1a, infile1b, infile2, infile3)
```

Arguments

toxval.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	

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
```

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

88 iris.cancer.clean

```
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/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

Description

create IRIS cancer clean source file from https://cfpub.epa.gov/ncea/iris/search/index.cfm by selecting cancer, oral and inhalation data, and toxicity value checkboxes.

Usage

```
iris.cancer.clean(infile)
```

Arguments

 iris.noncancer.clean 89

```
iris.noncancer.clean
```

create IRIS non cancer clean source file from iris_scrape_rfd_rfc 2020-05-27.xlsx and iris_scrape_woe 2020-05-27.xlsx (build using iris.scraper.R)

Description

create IRIS non cancer clean source file from iris_scrape_rfd_rfc 2020-05-27.xlsx and iris_scrape_woe 2020-05-27.xlsx (build using iris.scraper.R)

Usage

```
iris.noncancer.clean(infile1, infile2)
```

Arguments

infile1	The input file/iris/iris_files/iris_scrape_rfd_rfc 2020-05-27.xlsx
infile2	The input file/iris/iris_files/iris_scrape_woe 2020-05-27.xlsx

iris.scraper

Scrape the IRIS website

Description

Scrape the IRIS website

Usage

```
iris.scraper()
```

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)

```
load.dsstox()
```

90 log_message

Description

Function to load Clowder document information to database.

Usage

```
load_clowder_document_name(toxval.db, apiKey, clowder_dataset)
```

Arguments

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

apiKey The API key required for a user to access the Clowder dataset, prefix the apiKey

value with "?key="

clowder_dataset

A character string for the dataset name First create a table in source db with clowder document name and record source hash Update missing document names in toxval v9 record source table using data from clowder table apiKey="", clow-

der dataset="CCTE ToxValDB PDFs"

source.db The version of toxval source into which clowder data is loaded.

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

```
\label{log_df} \mbox{Dataframe to which the log information will be appended} \\ \mbox{message\_df\_col}
```

New message to add

map.chemical.to.dsstox 91

```
map.chemical.to.dsstox
```

Perform the DSSTox mapping

Description

Perform the DSSTox mapping

Usage

```
map.chemical.to.dsstox(toxval.db, verbose = T)
```

Arguments

toxval.db The version of toxvaldb to use.

verbose If TRUE, print out extra diagnostic messages

```
map.chemical.to.dsstox.by.source
```

Perform the DSSTox mapping

Description

Perform the DSSTox mapping

Usage

```
map.chemical.to.dsstox.by.source(toxval.db, source, verbose = T)
```

Arguments

toxval.db The version of toxvaldb to use.

verbose If TRUE, print out extra diagnostic messages

```
\begin{tabular}{ll} \verb|map.chemical.to.dsstox.ecotox| & \textit{use name and dtxsid pulled from ECOTOX in source\_chemical for eco----} \\ \end{tabular}
```

Description

use name and dtxsid pulled from ECOTOX in source_chemical for ecotox

Usage

```
map.chemical.to.dsstox.ecotox(toxval.db, source, verbose = T)
```

Arguments

toxval.db The version of toxvaldb to use.

verbose If TRUE, print out extra diagnostic messages

```
map.chemical_list.to.dsstox
```

Perform the DSSTox mapping

Description

Perform the DSSTox mapping

Usage

```
map.chemical_list.to.dsstox(toxval.db, verbose = T)
```

Arguments

toxval.db The version of toxvaldb to use.

verbose If TRUE, print out extra diagnostic messages

```
map.hash.record.clowder.document_name
```

Replace record_source_hash with clowder record_source_hash by mapping using document names

Description

Replace record_source_hash with clowder record_source_hash by mapping using document names

Usage

```
map.hash.record.clowder.document_name(toxval.db, apiKey, clowder_dataset)
```

Arguments

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

apiKey The API key required for a user to access the Clowder dataset, prefix the apiKey

value with "?key="

clowder_dataset

A character string for the dataset name First create a table in source db with clowder document name and record source hash Update record_source_hash in toxval v9 record source table using data from clowder table apiKey="?key=d2547ff7-

83ee-4f4e-b7b8-9875a5b18a83", clowder_dataset="CCTE ToxValDB PDFs"

source.db The version of toxval source into which clowder data is loaded.

```
map.hash.record_source
```

Map the icf master sheet hash to record source table hash

Description

Map the icf master sheet hash to record source table hash

Usage

```
map.hash.record_source(toxval.db, source.db)
```

Arguments

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

Value

94 niosh.pdf.to.excel

```
map.hash.record_source.by.source
```

Map the icf master sheet hash to record source table hash

Description

Map the icf master sheet hash to record source table hash

Usage

```
map.hash.record_source.by.source(toxval.db, source)
```

Arguments

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

Value

The database will be altered

```
niosh.pdf.to.excel niosh.pdf.to.excel
```

Description

Conversion of NIOSH pdf to Excel file

Usage

```
niosh.pdf.to.excel(infile)
```

Arguments

infile

The input file ../niosh/niosh_files/CDC - Index of Chemicals - NIOSH Publications and Products.pdf

parse.effect.level 95

parse.effect.level Process the the string that has the qualifier, value and units

Description

Process the the string that has the qualifier, value and units

Usage

```
parse.effect.level(val)
```

Arguments

val

The string

Value

a list with three values: qualifier, value, units

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.

96 pprtv.ncea.load.all

poc.summary.plot Make a scatter plot of the relationship between info availability and Scientific Domain Metric

Description

Make a scatter plot of the relationship between info availability and Scientific Domain Metric

Usage

```
poc.summary.plot(to.file = F, sys.date, do.read = F)
```

Arguments

to.file If TRUE, print the graph to a file, else write to the screen

sys.date The date of the bin data Excel fileto read

do.read if TRUE, read in the source file and store in a global

pprtv.ncea.load.all

Load NEW PPRTV (NCEA) to toxval_source. The data is found in a series of files: ../pprtv_ncea/pprtv_ncea_files/assessments.xlsx ../pprtv_ncea/pprtv_ncea_files/assessment_study.xlsx ../pprtv_ncea/pprtv_ncea_files/reference.xlsx ../pprtv_ncea/pprtv_ncea_files/study.xlsx ../pprtv_ncea/pprtv_ncea_files/dose_reg2.csv ../pprtv_ncea/PPRTV_scrape2020-04-08.xlsx

Description

Load NEW PPRTV (NCEA) to toxval_source. The data is found in a series of files: ../pprtv_ncea/pprtv_ncea_files/assessmen ../pprtv_ncea/pprtv_ncea_files/assessment_study.xlsx ../pprtv_ncea/pprtv_ncea_files/reference.xlsx ../pprtv_ncea/pprtv_ncea_files/study.xlsx ../pprtv_ncea/pprtv_ncea_files/dose_reg2.csv ../pprtv_ncea/PPRTV_scrape2020-04-08.xlsx

Usage

```
pprtv.ncea.load.all(source.db)
```

Arguments

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

pprtv.ncea.scraper 97

pprtv.ncea.scraper Prepare the PPRTV data downloaded October 2018. Go to the web site https://hhpprtv.ornl.gov/quickview/pprtv.php

Description

Prepare the PPRTV data downloaded October 2018. Go to the web site https://hhpprtv.ornl.gov/quickview/pprtv.php

Usage

```
pprtv.ncea.scraper()
```

```
pprtv.ornl.load.all.new
```

Prepare all of the PPRTV data from files downloaded May 2020. Go to the web site https://hhpprtv.ornl.gov/quickview/pprtv_compare.php and download the individual files listed here. The combined data is in the file ../pprtv_ornl/pprtv_ornl_files/PPRTV_ORNL_noncancer.xlsx

Description

Prepare all of the PPRTV data from files downloaded May 2020. Go to the web site https://hhpprtv.ornl.gov/quickview/pprtv_and download the individual files listed here. The combined data is in the file ../pprtv_ornl/pprtv_ornl_files/PPRTV_ORNL_n

Usage

```
pprtv.ornl.load.all.new(filepath, verbose = F)
```

Arguments

filepath The input files are in path ../pprtv_ornl/pprtv_ornl_files

pprtv.ornl.scraper Prepare the PPRTV data downloaded October 2018. Go to the web site https://hhpprtv.ornl.gov/quickview/pprtv.php

Description

Prepare the PPRTV data downloaded October 2018. Go to the web site https://hhpprtv.ornl.gov/quickview/pprtv.php

```
pprtv.ornl.scraper()
```

98 reset.numeric

```
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

reset.numeric

Reset the numeric and units values to their original values

Description

Reset the numeric and units values to their original values

Usage

```
reset.numeric(toxval.db)
```

Arguments

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

Value

runInsert 99

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

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_psql

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 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

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 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

runStatement 101

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

Description

Run a SQL statement, such as an ALTER or UPDATE

Usage

```
runStatement(query, db, do.halt = F, verbose = 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

Value

None. SQL statement is run.

set.dtxsid Set the dtxsid values for all of the other tables

Description

Set the dtxsid values for all of the other tables

Usage

```
set.dtxsid(toxval.db, table, verbose = T)
```

Arguments

toxval.db The version of toxvaldb to use.
table the Database table to be updated

verbose If TRUE, print out extra diagnostic messages

102 set.hash.bcfbaf

```
set.dtxsid.by.source
```

Set the dtxsid values for all of the other tables

Description

Set the dtxsid values for all of the other tables

Usage

```
set.dtxsid.by.source(toxval.db, table, source, verbose = T)
```

Arguments

toxval.db The version of toxvaldb to use.
table the Database table to be updated

verbose If TRUE, print out extra diagnostic messages

set.hash.bcfbaf Set the hash in table bcfbaf

Description

Set the hash in table bcfbaf

Usage

```
set.hash.bcfbaf(toxval.db, do.reset = T)
```

Arguments

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

do.reset if TRUE, reset all hashes and start rom scratch. Otherwise only update empty

values

Value

```
set.hash.bcfbaf.by.source
```

Set the hash in table bcfbaf

Description

Set the hash in table bcfbaf

Usage

```
set.hash.bcfbaf.by.source(toxval.db, source, do.reset = T)
```

Arguments

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

do.reset if TRUE, reset all hashes and start rom scratch. Otherwise only update empty

values

Value

The database will be altered

```
set.hash.genetox_details
```

Set the hash in table genetox_details

Description

Set the hash in table genetox_details

Usage

```
set.hash.genetox_details(toxval.db, do.reset = T)
```

Arguments

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

do.reset if TRUE, reset all hashes and start rom scratch. Otherwise only update empty

values

Value

Description

Set the hash in table genetox_details

Usage

```
set.hash.genetox_details.by.source(toxval.db, source, do.reset = T)
```

Arguments

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

do.reset if TRUE, reset all hashes and start rom scratch. Otherwise only update empty

values

Value

The database will be altered

```
set.hash.record_source
```

Set the hash in table record_source

Description

Set the hash in table record_source

Usage

```
set.hash.record_source(toxval.db, do.reset = T)
```

Arguments

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

do.reset if TRUE, reset all hashes and start from scratch. Otherwise only update empty

values

Value

```
set.hash.record_source.by.source
Set the hash in table record_source
```

Description

Set the hash in table record_source

Usage

```
set.hash.record_source.by.source(toxval.db, source, reset = T)
```

Arguments

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

do.reset if TRUE, reset all hashes and start from scratch. Otherwise only update empty

values

Value

The database will be altered

```
set.hash.skin_eye Set the hash in table skin_eye
```

Description

Set the hash in table skin_eye

Usage

```
set.hash.skin_eye(toxval.db, do.reset = T)
```

Arguments

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

do.reset if TRUE, reset all hashes and start rom scratch. Otherwise only update empty

values

Value

106 set.hash.source

```
set.hash.skin_eye.by.source

Set the hash in table skin_eye
```

Description

Set the hash in table skin_eye

Usage

```
set.hash.skin_eye.by.source(toxval.db, source, do.reset = T)
```

Arguments

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

do.reset if TRUE, reset all hashes and start rom scratch. Otherwise only update empty

values

Value

The database will be altered

set.hash.source Set the hash in source table

Description

Set the hash in source table

Usage

```
set.hash.source(source.db, source, reset = F)
```

Arguments

source.db The source database version where data is getting altered (eg: dev_toxval_source_v4).

The table in source where the hash data is getting altered.

do.reset if TRUE, reset all hashes and start from scratch. Otherwise only update empty

values

Value

set.hash.toxval

set.hash.toxval

Set the hash in table toxval

Description

Set the hash in table toxval

Usage

```
set.hash.toxval(toxval.db, do.reset = T)
```

Arguments

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

do.reset if TRUE, reset all hashes and start from scratch. Otherwise only update empty

values

Value

The database will be altered

```
set.hash.toxval.by.source
```

Set the hash in table toxval

Description

Set the hash in table toxval

Usage

```
set.hash.toxval.by.source(toxval.db, source, reset = T)
```

Arguments

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

do.reset if TRUE, reset all hashes and start from scratch. Otherwise only update empty

values

Value

108 setPSQLDBConn

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

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_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

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.table.to.DAT

source.table.to.DAT
```

Description

Convert toxval source table to DAT format for loading to DAT application

Usage

```
source.table.to.DAT(source.db, source_table, limit = 1e+06, sample_p = NA)
```

Arguments

source.db The version of toxval source to use.

source_table The name of toxval source table to use.

limit Excel file grouping limit (default is max XLSX row limit)

sample_p Percentage of records to sample down to

source The name of toxval source to use.

Value

Processed source table to DAT format cached and returned.

```
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 111

```
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

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

res 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",
```

source_prep_and_load 113

```
name.col = "name",
  verbose = F
)
```

Arguments

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

Source.db The source database version

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 the column containing has chemical name

If TRUE, write out diagnostic messages

Value

verbose

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)
```

114 source_set_defaults

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 115

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
```

116 toxval.init.db

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

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

toxval.load.alaska_dec 117

```
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
```

118 toxval.load.atsdr.pfas

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.

```
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

120 toxval.load.cal_dph

```
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

toxval.load.cancer 121

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 ../cancer_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.chemical.list

Load The chemical lists to toxval. All Excel files in the folder ../chemicals/for_load/ are loaded. The must have the columns casrn, name, list_name

Description

Load The chemical lists to toxval. All Excel files in the folder ../chemicals/for_load/ are loaded. The must have the columns casrn, name, list_name

Usage

```
toxval.load.chemical.list(toxval.db, verbose = T)
```

Arguments

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

verbose If TRUE, print debugging messages

toxval.load.chemical.list.by.source

Load The chemical lists for corresponding sources to toxval. All Excel files in the folder ../chemicals/for_load/ are loaded. The must have the columns casrn, name, list_name

Description

Load The chemical lists for corresponding sources to toxval. All Excel files in the folder ../chemicals/for_load/ are loaded. The must have the columns casrn, name, list_name

Usage

```
toxval.load.chemical.list.by.source(toxval.db, source, verbose = T)
```

Arguments

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

verbose If TRUE, print debugging messages

```
toxval.load.chemical.list.ecotox
```

Load The chemical lists for corresponding sources to toxval. All Excel files in the folder ../chemicals/for_load/ are loaded. The must have the columns casrn, name, list_name

Description

Load The chemical lists for corresponding sources to toxval. All Excel files in the folder ../chemicals/for_load/ are loaded. The must have the columns casrn, name, list_name

Usage

```
toxval.load.chemical.list.ecotox(toxval.db, source, verbose = T)
```

Arguments

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

verbose If TRUE, print debugging messages

toxval.load.chiu 123

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.

log If TRUE, send output to a log file

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.

124 toxval.load.dod

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.

log If TRUE, send output to a log file

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.

toxval.load.dod.ered 125

```
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.

log If TRUE, send output to a log file

Description

 $Load\ new_doe_table\ and\ new_doe_benchmarks_table\ from\ toxval_source\ to\ toxval$

Usage

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

Arguments

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

source.db The source database to use.

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

126 toxval.load.doe.ecorisk

```
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	on of toxval into w	hich the tables are loaded.
-----------------------	---------------------	-----------------------------

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

toxval.load.doe.pac 127

```
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.

128 toxval.load.efsa

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

source.db The source database to use.

toxval.load.efsa2

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.

130 toxval.load.fda_cedi

```
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

toxval.load.flex 131

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

Description

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

Usage

```
toxval.load.flex(toxval.db, verbose = F, only.new = F)
```

Arguments

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

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

only.new if TRUE only files where the sources is not alrady in the database will be loaded

```
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

toxval.load.hawc 133

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 = 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_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.

134 toxval.load.healthcanada

```
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.

log If TRUE, send output to a log file

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 ve	ersion of toxval int	to which the tab	oles are loaded.
------------------	----------------------	------------------	------------------

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

toxval.load.heast

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.

log If TRUE, send output to a log file

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.

136 toxval.load.initial

```
{\tt toxval.load.hpvis} \quad \textit{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
log	If TRUE, send output to a log file

```
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 137

toxval.load.iris Load new_iris_noncancer and new_iris_cancer from toxval_source to toxval

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

138 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 139

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.

140 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 141

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

 $\verb"source.db" The source database"$

```
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 = 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.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 143

```
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.

log If TRUE, send output to a log file

```
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

144 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 = 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.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

```
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

146 toxval.load.toxrefdb3

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 = 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.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 147

```
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

log If TRUE, send output to a log file

```
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

toxval.qc.step.1

```
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 are loaded.

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

log If TRUE, send output to a log file

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 149

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

 $toxval. source. add. timestamps \\ toxval. source. add. timestamps$

Description

get chemical info from source db tables

Usage

```
toxval.source.add.timestamps(source.db)
```

Arguments

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

Value

None. SQL statements are executed to add timestamp columns.

```
toxval.source.map.chemicals

toxval.source.map.chemicals
```

Description

push ChemReg curated chemicals to toxval_source db tables

Usage

```
toxval.source.map.chemicals(source.db, input.path, curated.path)
```

Arguments

```
source.db The version of toxval source database to use.
input.path Path to folder with original chemical lists
curated.path Path to folder with curated chemical lists
```

Value

None. SQL statements are executed.

```
toxval.source.map.chemicals.combined toxval.source.map.chemicals.combined
```

Description

push ChemReg curated chemicals to toxval_source db tables

Usage

```
toxval.source.map.chemicals.combined(
  source.db,
  input.path,
  curated.path,
  match.raw = FALSE
)
```

Arguments

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

input.path Path to folder with original chemical lists

curated.path Path to folder with curated chemical lists

match.raw Boolean whether to match by raw name/casrn values (Default FALSE)
```

toxval.summary.stats 151

Value

None. SQL statements are executed.

```
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

Index

```
* cas functions
                                        export.missing.strains, 24
   cas_checkSum, 8
                                        export.pod.summary, 24
                                        export.record_source, 25
build_echa_echemportal_api_dict,
                                        export.skin_eye, 25
       8
                                        export.source_chemical, 26
                                        export.toxval_dictionary, 26
cas checkSum, 8
cas_detect, 8, 9
                                        fill.chemical, 27
chem.check, 9
                                        fill.chemical.by.source, 27
chem.check.v2, 10
                                        fill.chemical_source_index, 28
clean.last.character, 11
                                        fill.toxval.defaults, 28
clean.toxval.by.source, 11
                                        fill.toxval.defaults.global, 29
clowder_document_list, 12
                                        fill.toxval.defaults.global.by.source,
clowder_id_prep.v3, 12
                                               29
compare.pfas_150_sem.to.hawc, 13
                                        fix.all.param, 30
                                        fix.all.param.by.source, 30
contains, 13
                                        fix.all.param.new, 31
echemportal.prep.v2, 14
                                        fix.all.param.new.by.source, 31
echemportal.prep.v2.step2, 14
                                        fix.casrn, 32
echemportal.prep.v2.step3, 14
                                        fix.clowder_id.by.source, 32
ecotox.datahub.to.file, 15
                                        fix.clowder_id.by.toxval, 33
efsa.clean, 15
                                        fix.critical_effect, 33
efsa.dict.prep, 16
                                        fix.critical_effect.icf.by.source,
efsa.prep, 16
                                                34
export.all.by.source, 17
                                        fix.empty, 34
export.all.by.source.for.release,
                                        fix.empty.by.source, 35
                                        fix.empty.hyphen.record_source.by.source,
export.all.by.source.pfas, 18
export.all.with.references, 18
                                        fix.empty.record_source, 36
export.bcfbaf, 19
                                        fix.empty.record_source.by.source,
export.cancer.summary, 19
                                                36
                                        fix.exposure_form, 37
export.chemicals, 20
export.dsstox, 20
                                        fix.exposure_form.by.source, 37
export.dsstox.mol.wt, 20
                                        fix.exposure_method.and.form.by.source,
export.echa.repeats, 21
export.final.params, 21
                                        fix.exposure_route.by.type, 38
export.genetox_details, 22
                                        fix.exposure_route.by.type.new,
export.genetox_summary, 22
export.missing.rac, 23
                                        fix.exposure_route.by.type.new.by.source,
export.missing.rac.by.source, 23
```

INDEX 153

fix.generation.by.source, 39	heast.load.all,61
fix.human_eco,40	hess_record_url_from_clowder,62
fix.human_eco.by.source, 40	
fix.hyphen.by.source, 41	ig.summary.plot, 62
fix.non_ascii,41	import.dictionary, 63
fix.non_ascii.v2,42	import.driver, 63
fix.priority_id, 42	import.source.info,64
fix.priority_id.by.source, 43	import.source.info.by.source, 64
fix.qa_status, 43	import_actor_source,65
fix.qa_status.by.source,44	<pre>import_atsdr_pfas_2021_source,65</pre>
fix.qc_status.by.source, 44	import_atsdr_pfas_source,66
fix.risk_assessment_class, 45	import_atsdr_source,66
fix.risk_assessment_class.all.source,	import_caloehha_source,67
45	import_chiu_source,67
fix.risk_assessment_class.by.source,	import_copper_source, 68
46	import_cosmos_source, 69
fix.single.param, 46	<pre>import_dod_ered_source, 69</pre>
fix.single.param.by.source, 47	import_dod_source, 70
	<pre>import_doe_benchmarks_source, 70</pre>
fix.single.param.new, 47	<pre>import_doe_source,71</pre>
fix.single.param.new.by.source,	<pre>import_echa3_source,71</pre>
48	<pre>import_echa_echemportal_api_source</pre>
fix.species, 48	72
fix.species.by.source, 49	<pre>import_echa_echemportal_source,</pre>
fix.species.ecotox.by.source, 49	73
fix.species.v2,50	<pre>import_echa_iuclid_source, 73</pre>
fix.species_ecotox, 50	import_echa_source, 74
fix.strain.by.source, 51	import_efsa2_source,74
fix.strain.v2,51	import_efsa_source, 75
fix.toxval_numeric_qualifier, 52	:
fix.toxval_numeric_qualifier.by.sourc	'mport_flex_source, 76
32	import_generic_source, 77
fix.units, 53	import_hawc_pfas_150_source,77
fix.units.by.source, 53	import_hawc_pfas_430_source,78
fix.units.new, 54	import_hawc_source, 79
fix.units.new.by.source, 55	import_health_canada_source, 79
fix.units.testmw, 56	import_heast_source, 80
format_rsl_excel, 56	import_hess_source, 80
	import_hpvis_source, 81
generate.originals,57	import_iris_source, 81
get.chemical.info.by.source, 57	import_lanl_source, 82
get.chemical.info.by.source.combined,	
58	import_opp_source, 83
get.cid.list.toxval,58	import_oppt_source, 83
get.cid.list.toxval.ecotox,59	import_penn_source, 84
get.clowder.file.maps,59	import_pfas_150_sem_v2_source, 84
get_clowder_docList, 61	<pre>import_pprtv_ncea_source, 85</pre>
getDBConn, 60	import_pprtv_ornl_source, 85
getPSQLDBConn, 60	import_rsl_source, 86

154 INDEX

import_rsl_source_info,87	set.hash.record_source.by.source,
import_test_source, 87	105
import_wignall_source, 88	set.hash.skin_eye,105
iris.cancer.clean, 88	set.hash.skin_eye.by.source,106
iris.noncancer.clean, 89	set.hash.source, 106
iris.scraper,89	set.hash.toxval, 107
is.cas,9	set.hash.toxval.by.source, 107
	set_clowder_id, 109
load.dsstox, 89	setDBConn, 108
load_clowder_document_name, 90	setPSQLDBConn, 108
$\log_{message}, 90$	source.size, 109
	source.table.to.DAT, 110
map.chemical.to.dsstox,91	source_chemical.duplicates, 110
<pre>map.chemical.to.dsstox.by.source,</pre>	source_chemical.ecotox, 111
91	source_chemical.process, 111
map.chemical.to.dsstox.ecotox, 92	source_chemical.toxrefdb, 112
<pre>map.chemical_list.to.dsstox, 92</pre>	source_prep_and_load, 113
map.hash.record.clowder.document_nam	
93	species.mapper, 115
map.hash.record_source, 93	
map.hash.record_source.by.source,	toxval.check.source_chemical, 115
94	toxval.config, 116
	toxval.init.db, 116
niosh.pdf.to.excel,94	toxval.load.alaska_dec,117
_	toxval.load.all, 117
parse.effect.level, 95	toxval.load.atsdr, 118
pfas.by.source,95	toxval.load.atsdr.pfas, 118
poc.summary.plot,96	toxval.load.atsdr.pfas.2021,119
pprtv.ncea.load.all, 96	toxval.load.bcfbaf, 119
pprtv.ncea.scraper, 97	toxval.load.cal_dph, 120
pprtv.ornl.load.all.new,97	toxval.load.caloehha, 120
pprtv.ornl.scraper,97	toxval.load.cancer, 121
printCurrentFunction, 98	toxval.load.chemical.list, 121
,	toxval.load.chemical.list.by.source
reset.numeric, 98	122
runInsert, 99	toxval.load.chemical.list.ecotox,
runInsertTable, 99	122
runQuery, 100	toxval.load.chiu, 123
runQuery_psql, 100	toxval.load.copper, 123
runStatement, 101	toxval.load.cosmos, 124
,	toxval.load.dod, 124
set.dtxsid, 101	toxval.load.dod.ered, 125
set.dtxsid.by.source, 102	toxval.load.doe, 125
set.hash.bcfbaf, 102	toxval.load.doe.benchmarks, 126
set.hash.bcfbaf.by.source, 103	toxval.load.doe.ecorisk, 126
set.hash.genetox_details, 103	toxval.load.doe.pac, 127
set.hash.genetox_details.by.source,	toxval.load.echa.echemportal.api,
104	127
set.hash.record_source, 104	toxval.load.ecotox, 128

INDEX 155

```
toxval.load.efsa, 128
                                        webchem, 9
toxval.load.efsa2, 129
toxval.load.envirotox, 129
toxval.load.epa_aegl, 130
toxval.load.fda_cedi, 130
toxval.load.flex, 131
toxval.load.generic, 131
toxval.load.genetox, 132
toxval.load.genetox_details, 132
toxval.load.hawc, 133
toxval.load.hawc pfas 150, 133
toxval.load.hawc_pfas_430,134
toxval.load.healthcanada, 134
toxval.load.heast, 135
toxval.load.hess, 135
toxval.load.hpvis, 136
toxval.load.initial, 136
toxval.load.iris, 137
toxval.load.mass_mmcl, 137
toxval.load.new ecotox, 138
toxval.load.niosh, 138
toxval.load.opp, 139
toxval.load.oppt, 139
toxval.load.osha_air_limits, 140
toxval.load.ow_dwsha, 140
toxval.load.penn, 141
toxval.load.penn_dep, 141
toxval.load.pfas_150_sem_v2, 142
toxval.load.postprocess, 142
toxval.load.pprtv.ncea, 143
toxval.load.pprtv.ornl, 143
toxval.load.rsl, 144
toxval.load.skin.eye, 144
toxval.load.source_chemical, 145
toxval.load.species, 145
toxval.load.test, 146
toxval.load.toxrefdb3,146
toxval.load.usgs_hbsl, 147
toxval.load.who_ipcs, 147
toxval.load.wignall, 148
toxval.qc.step.1, 148
toxval.set.mw, 149
toxval.source.add.timestamps, 149
toxval.source.map.chemicals, 150
toxval.source.map.chemicals.combined,
       150
toxval.summary.stats, 151
toxval_source.hash.and.load, 151
```