toxvaldbBMDh

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Title Calculates BMDh Values From Records in ToxValDB		
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Description This package extracts data from the ToxValDB database, filters it for redundant records (this redundancy should be reduced in later versions), and calculates study-level and chemical-level BMD. To run the entire process, uses the functions export.for.bmdh(), filter.for.bmdh(), bmd.per.study(), bmd.per.chemical() and bmdh.percentile.plot(). The function driver() runs all of the methods sequentially. The last function provides the best percentile to use. All of the input and output data lives in the data/ folder		
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bmdh.aurisano.check.plot

bmdh.aurisano.check.plot

Description

Plot the difference between the Aurisano and current BMDh values

Usage

```
bmdh.aurisano.check.plot(
  to.file = FALSE,
  toxval.db = "res_toxval_v95",
  sys.date = Sys.Date()
)
```

bmdh.cumdist.plot 3

Arguments

to.file If TRUE, send the plot to a file

toxval.db Database version

sys.date The date of the database export

Details

DETAILS

Value

None; writes plot to PDF

See Also

```
read.xlsx ggplot, aes, labs, geom_point, ggtheme, scale_continuous, ggsave dev
```

Examples

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

bmdh.cumdist.plot

bmdh.cumdist.plot

Description

Plot the cumulative distribution of number of studies

Usage

```
bmdh.cumdist.plot(
  to.file = F,
  toxval.db = "res_toxval_v95",
  sys.date = Sys.Date()
)
```

Arguments

to.file If TRUE, send the plot to a file

toxval.db Database version

sys.date The date of the database export

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Details

DETAILS

Value

writes a plot to a file

See Also

```
read.xlsx ggplot, aes, labs, stat_ecdf, ggtheme, lims, ggsave ggarrange dev
```

Examples

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

bmdh.per.chemical

bmdh.per.chemical

Description

Calculate BMDh values one per chemical

Usage

Arguments

toxval.db Database name

run_name The desired name for the output directory (Default: current date)

regulatory.sources

This is the list of sources that will be used to select the #' optimal quantile to use for selecting the final chemical-level BMDh.

bmdh.per.study 5

Details

Calculates one BMDh value per chemical. This is done by taking various percentiles of the distribution of the BMDh values and building a table with one column per percentile per chemical. The values are calibrated against regulatory values. The list of high-quality, regulator sources is given as one of the calling arguments.

Value

Write a file with the results: toxval_PODs_for_BMDh chemical level toxval.db sys.date.xlsx

See Also

```
read.xlsx, createStyle, write.xlsx sd, quantile
```

Examples

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

bmdh.per.study

bmdh.per.study

Description

Calculate the BMDh values per study

Usage

```
bmdh.per.study(toxval.db, run_name = Sys.Date())
```

Arguments

toxval.db Database name

run_name The desired name for the output directory (Default: current date)

Details

Calculates one BMDh value per study using the Aurisano algorithm. Because EPA has not fully developed the mapping from critical effects in ToxValDB to standardized effects, teh values from Aurisano are used where records match. Aurisano used ToxValDB 9.1, whereas 9.5 is used here. There is also code here to do the other required mappings, and thos may need to be updated. For records in both the old and new databases, an on-the-fly plot is produced to show the corresponded between study-level BMDh values.

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Value

Write a file with the results: toxval_PODs_for_BMDh toxval.db sys.date.xlsx

See Also

```
read.xlsx, createStyle, write.xlsx plot.default
```

Examples

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

bmdh.percentile.plot bmdh.percentile.plot

Description

Plot the BMDs vs the regulatory values for different percentiles and determine the best fit

Usage

```
bmdh.percentile.plot(
  to.file = FALSE,
  toxval.db,
  run_name = Sys.Date(),
  minstudies = 3,
  cutoff.logsd = 2
)
```

Arguments

to.file If TRUE, send the plot to a file

toxval.db Database name

run_name The desired name for the output directory (Default: current date)

minstudies - only chemicals with this minimum number of studies will be used in the cal-

culation

cutoff.logsd Only chemicals with their log SD of BMDh values will be used in the calculation

Details

Helps determine the optimal percentile. The output file shows the fit statistics for different percentiles, and one should select the one with the lowest RMSE and highest R2.

Value

Write a file with the results: toxval_PODs_for_BMDh chemical level toxval.db sys.date.xlsx

See Also

```
read.xlsx,write.xlsxlmcharacter(0) ggplot, aes, labs, geom_point, ggtheme, facet_grid,
lims, geom_segment, ggsave dev
```

Examples

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

Description

Attempts to remap previously-mapped toxicological_effect_category values to DCAP entries

Usage

```
check_dcap_toxicological_effect_category_mappings(
  toxval.db,
  get_suggestions = TRUE,
  input_file = "",
  output_dir = ""
)
```

Arguments

```
toxval.db The version of ToxVal to use get_suggestions

Whether to provide mapping suggestions (Default: TRUE) input_file The file to pull missing toxicological_effect_category from. output_dir The folder used to write output to
```

Details

The output Excel files are as follows: -dcap_mappings_identified.xlsx: All toxicological_effect_categories that could be confidently remapped - dcap_mappings_still_missing.xlsx: Full data for entries missing categorizations - dcap_missing_categorization.xlsx: Just toxicological_effect, study_type values missing categorizations - dcap_mapping_suggestions.xlsx: Mapping suggestions based on close, but not exact, matches

8 convert.fields.to.json

Value

None; output is written to Excel files

```
convert.fields.to.json

convert.fields.to.json
```

Description

Combine non-ID columns from audit table into JSON format for audit storage

Usage

```
convert.fields.to.json(in_dat)
```

Arguments

in_dat

data to translate to JSON format

Details

DETAILS

Value

Values in JSON format

See Also

```
summarise, select, bind toJSON, fromJSON
```

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

```
convert\_get\_conversion\_factor\\ convert\_get\_conversion\_factor
```

Description

A helper function to convert input values to desired units.

Usage

```
convert_get_conversion_factor(conv_factor = 1)
```

Arguments

conv_factor

Conversion factor to use (such as Molecular weight, tissue Density, etc.)

Details

DETAILS

Value

List of conversion factors

Examples

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

convert_units

 $FUNCTION_TITLE$

Description

A helper function to convert input values to desired units.

Usage

```
convert_units(x, units, desired, conv_factor = NA)
```

10 dcap.counts

Arguments

x Numeric to be convertedunits Original units to be converted

desired Desired units to convert the input value into

conv_factor Conversion factor to use (such as Molecular weight, tissue Density, etc.)

overwrite_units

Boolean to overwrite the 'units' with desired units.

Details

DETAILS

Value

OUTPUT_DESCRIPTION

Examples

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

dcap.counts

dcap.counts

Description

Calculate some stats for DCAP

Usage

```
dcap.counts(toxval.db, run_name = Sys.Date())
```

Arguments

toxval.db Database name

run_name The desired name for the output directory (Default: current date)

Details

Gets some statistics for the DCAP project off of the current ToxValDB export

driver 11

Value

Write a file with the filtered results:ToxValDB for BMDh filtered toxval.db sys.date.xlsx

See Also

```
read.xlsx, write.xlsx
```

Examples

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

driver

driver

Description

Run all of the calculations to go from database export to calculation of final BMDh values

Usage

```
driver(
  toxval.db,
  run_name = Sys.Date(),
  run.export = TRUE,
  include.pesticides = FALSE,
  include.drugs = FALSE,
  include.epa_dws = TRUE,
  include.food_add = FALSE,
  reset.study_group = FALSE
)
```

Arguments

Flag to include EPA DWS in output or not

12 export.for.bmdh

Details

DETAILS

Value

None

Examples

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

export.for.bmdh

export.for.bmdh

Description

Export records required for calculating BMDh values.

Usage

```
export.for.bmdh(
  toxval.db,
  include.pesticides = FALSE,
  include.drugs = FALSE,
  include.epa_dws = TRUE,
  include.food_add = FALSE,
  reset.study_group = FALSE,
  run_name = Sys.Date()
)
```

Arguments

```
toxval.db Database version include.pesticides Flag to include pesticides in output or not include.drugs Flag to include drugs in output or not
```

```
include.epa_dws
Flag to include EPA DWS in output or not
include.food_add
Flag to include food additives in output or not
reset.study_group
Flag to reset study_group
run_name
The desired name for the output directory (Default: current date)
```

Details

Exports all of the data required for the BMDh calculations. The main query may need to be modified to extract more columns if needed for the final application. Certain sources have been excluded because they have a high percentage of read-across values. Species are filtered to only include Human, Dog, Mouse, Rat and Rabbit. If more species are to be included, then allometric scaling factors for those need to added to the function bmd.per.study().

Value

Write a file with the results: ToxValDB for BMDh toxval.db Sys.Date().xlsx

See Also

```
createStyle, write.xlsx
```

Examples

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

Description

Export records required for managing the critical effect categories for the BMD calculations.

Usage

```
export.for.toxicological_effect_mapping(
  toxval.db = "res_toxval_v95",
  user = "rjudson",
  password
)
```

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Arguments

toxval.db Database version

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

in the function setDBConn().

password The user's MySQL database password.

Details

Exports all of the data required for performing the critical effect mapping for the BMDh calculations

Value

Write a file with the results: ToxValDB for BMDh toxval.db Sys.Date().xlsx

See Also

```
createStyle, write.xlsx
```

Examples

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

filter.pods

filter.pods

Description

Filter values for BMDh according to specified POD rules

Usage

```
## S3 method for class 'pods'
filter(toxval.db, run_name = Sys.Date())
```

Arguments

toxval.db Database name

run_name The desired name for the output directory (Default: current date)

Details

Filtering steps differ between authoritative and non-authoritative sources

filter.summary 15

Value

None; filtered results are recorded in Excel file

See Also

```
read.xlsx, createStyle, write.xlsx
```

Examples

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

filter.summary

filter.summary

Description

Summarize the filtering steps

Usage

```
## S3 method for class 'summary'
filter(toxval.db, run_name = Sys.Date(), do.load = TRUE)
```

Arguments

toxval.db Database name

run_name The desired name for the output directory (Default: current date)

do.load Whether to load data from Excel, Default: TRUE

Details

Filters where multiple NOEL/NOEL etc. exist. For each study_group this will select the highest NO(A)EL below the lowest LO(A)EL and the lowest LO(A)EL. In all cases, all BMDx values are included

Value

Write a file with the filtered results: Tox ValDB for BMDh LEL NEL multiNOEL filtered tox val. db sys.date.xlsx

See Also

```
read.xlsx, createStyle, write.xlsx
```

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Examples

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

fix.replace.unicode

fix.replace.unicode

Description

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

Usage

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

Arguments

df

Character vector to check/replace unicode symbols.

Details

DETAILS

Value

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

See Also

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

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

fix.study_group 17

fix.study_group

Set the study_group field

Description

Set the study_group field

Usage

```
fix.study_group(df)
```

Arguments

df

Input dataframe to set study_group

Value

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

```
{\tt get.conceptual\_model.by.toxicological\_effect\_category} \\ {\tt get.conceptual\_model.by.toxicological\_effect\_category}
```

Description

Get the conceptual model based on toxicological_effect_category

Usage

```
get.conceptual_model.by.toxicological_effect_category(df)
```

Arguments

df

Input dataframe of study_type and toxicological_effect data.

Details

DETAILS

Value

DataFrame map of models by toxicological_effect and study_type

See Also

```
select, distinct, mutate, context, case_when, mutate-joins, rename, across, reexports, group_by, na_if separate_rows, replace_na str_trim read_delim, cols
```

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Examples

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

getDBConn

getDBConn

Description

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

Usage

```
getDBConn()
```

Details

DETAILS

Value

print the database connection information

Examples

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

get_chemcial_index

get_chemical_index

Description

Generate a chemical index based on ToxVal DTXSID list and QSAR Ready Smiles.

Usage

```
get_chemcial_index(input_toxval_file, input_qsar_file)
```

init.current.run.directory 19

Arguments

Details

DETAILS

Value

Combined chemical index dataframe. A CSV file is also written to the input subfolder.

See Also

```
read_delim, cols, write_delim select, mutate-joins, distinct, c("rowwise", "rowwise"),
mutate, group_by map digest
```

Examples

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

Description

Initialize output directory for current driver run

Usage

```
init.current.run.directory(run_name = Sys.Date())
```

Arguments

run_name

The desired name for the output directory (Default: current date)

Details

DETAILS

20 pod.per.chemical

Value

None; new directory is created

Examples

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

pod.per.chemical

pod.per.chemical

Description

Explore different methods for calculating PODs

Usage

```
pod.per.chemical(toxval.db = "res_toxval_v95", sys.date = Sys.Date())
```

Arguments

toxval.db	The version of ToxValDB to use
sys.date	Date of the most recent data export #' Make the rule #' filter LOELs when NOELs are present for the same study #' filter out redundant values for the same study group #' Perform the allometric scaling
t2 scale.mat	PARAM_DESCRIPTION PARAM DESCRIPTION

Details

Explore different methods for calculating PODs This uses the same input as the function bmdh.perstudy / bmdh.per.chemical

Value

Writes output to file

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

pod.per.chemical.eco 21

Description

Calculate the eco PODs

Usage

```
pod.per.chemical.eco(toxval.db = "res_toxval_v95", sys.date = Sys.Date())
```

Arguments

toxval.db The version fo the ToxValDB to use sys.date The date of the database export

Details

DETAILS

Value

Writes output to file

See Also

```
read.xlsx, write.xlsx quantile, sd
```

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

22 pod.rule.maker

pod.rule.maker

pod.rule.maker

Description

Function to create/choose rule based on POD inputs

Usage

```
pod.rule.maker(
  toxval,
  hra.sources,
  rule.name = "Rule 3",
  rule.stype = "chronic",
  rule.ttype = "LO(A)EL, NO(A)EL, BMD",
  stype.list = c("chronic"),
  ttype.list = c(loel.types, noel.types, bmdl.types)
)
```

Arguments

```
toxval Input dataframe of ToxVal data.

hra.sources Human Risk Assessment source list

rule.name PARAM_DESCRIPTION, Default: 'Rule 3'

rule.stype PARAM_DESCRIPTION, Default: 'chronic'

rule.ttype PARAM_DESCRIPTION, Default: 'LO(A)EL, NO(A)EL, BMD'

stype.list PARAM_DESCRIPTION, Default: c("chronic")

ttype.list PARAM_DESCRIPTION, Default: c(loel.types, noel.types, bmdl.types)
```

Details

DETAILS

Value

Modified version of input toxval dataframe.

See Also

```
quantile, sd
```

printCurrentFunction 23

Examples

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

printCurrentFunction printCurrentFunction

Description

Print the name of the current function

Usage

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

Arguments

comment.string An optional string to be printed

Details

DETAILS

Value

None

See Also

flush.console

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

24 property.counter

property.counter

property.counter

Description

Count proerties of records

Usage

```
property.counter(toxval.db = "res_toxval_v95", sys.date = Sys.Date())
```

Arguments

toxval.db Database version

sys.date The date of the database export

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

in the function setDBConn().

password The user's MySQL database password.

Details

DETAILS

Value

Write a file with the results: ToxValDB for BMDh toxval.db Sys.Date().xlsx

See Also

```
read.xlsx, write.xlsx, createStyle
```

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

runQuery 25

runQuery runQuery

Description

Runs a database query and returns a result set

Usage

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

Arguments

query a properly formatted SQL query as a string

db the name of the database

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

Details

DETAILS

Value

Query results

See Also

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

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

```
source_hash_vectorized
source_hash_vectorized
```

Description

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

Usage

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

Arguments

res The data frame to be processed

hashing_cols Optional list of columns to use for generating source_hash

Details

DETAILS

Value

Input dataframe with new source_hash field

See Also

```
digest distinct
```

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

split.species.list 27

```
split.species.list Split species list
```

Description

Split species lists into multiple rows

Usage

```
## S3 method for class 'species.list'
split(df)
```

Arguments

df

Input dataframe with species lists to split

Details

DETAILS

Value

Modified input df with split species lists into multiple rows

See Also

```
mutate, case_when, filter, bind_rows, group_by, summarise separate_rows str_trim, case
```

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

28 studies.per.chemical

```
studies.per.chemical studies.per.chemical
```

Description

Calculate some stats for DCAP

Usage

```
studies.per.chemical(toxval.db, run_name = Sys.Date())
```

Arguments

toxval.db Database name

run_name The desired name for the output directory (Default: current date)

Details

Gets the number of studies per chemical from the current ToxValDB export

Value

Write a file with the filtered results:ToxValDB for BMDh filtered toxval.db sys.date.xlsx

See Also

```
read_xlsx, write_xlsx
```

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

study_group.multichem 29

```
study\_group.multichem \ \ \textit{study\_group.multichem}
```

Description

Find study groups that span multiple chemicals

Usage

```
study_group.multichem(toxval.db, run_name = Sys.Date())
```

Arguments

toxval.db Database name

run_name The desired name for the output directory (Default: current date)

Details

DETAILS

Value

Write a file with the filtered results: Tox ValDB for BMDh LEL NEL multiNOEL filtered tox val. db sys.date.xlsx

See Also

```
read.xlsx, createStyle, write.xlsx
```

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

```
toxicological\_effect\_source\\ toxicological\_effect\_source
```

Description

Find the source for odd critical effect chunks.

Usage

```
toxicological_effect_source(toxval.db = "res_toxval_v95", user, password)
```

Arguments

toxval.db Database version

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

in the function setDBConn().

password The user's MySQL database password.

Details

DETAILS

Value

Writes output to file

See Also

```
read.xlsx, write.xlsx
```

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

toxval.redundancies 31

toxval.redundancies

toxval.redundancies

Description

Detect potential redundancies in ToxValDB.

Usage

```
toxval.redundancies(toxval.db = "res_toxval_v95", user, password)
```

Arguments

toxval.db Database version

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

in the function setDBConn().

password The user's MySQL database password.

Details

DETAILS

Value

Write a file with the results

See Also

```
createStyle, write.xlsx
```

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

```
toxval.source.import.dedup

toxval.source.import.dedup
```

Description

Perform deduping on data before it is sent to toxval_source

Usage

```
toxval.source.import.dedup(
  res,
  dedup_fields = NULL,
  hashing_cols = NULL,
  delim = " |::| "
)
```

Arguments

res dataframe containing the source data to dedup

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

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

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

Details

DETAILS

Value

dataframe containing deduped source data

See Also

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

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

toxvaldb.statplots 33

toxvaldb.statplots

toxvaldb.statplots

Description

Plot statistics for ToxValDB for DCAP sources

Usage

```
toxvaldb.statplots(to.file = FALSE, toxval.db, run_name = Sys.Date())
```

Arguments

to.file Whether to write plots to file or simply view them, Default: F

toxval.db Database name

run_name The desired name for the output directory (Default: current date)

dir The directory where the lists are stored

Details

DETAILS

Value

None; plots are generated

See Also

read.xlsx ggplot, aes, labs, geom_boxplot, scale_continuous, scale_manual, coord_flip,
ggtheme, theme, element, geom_jitter, geom_freqpoly, facet_wrap, lims, ggsave fct_rev
reorder.default arrangeGrob dev

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

write_dcap_summary

write_dcap_summary

write_dcap_summary

Description

Output summary reports containing chemical and key field information

Usage

```
write_dcap_summary(toxval.db, sys.date = Sys.Date())
```

Arguments

toxval.db

The version of ToxVal to use

sys.date

The date of the export to use, Default: Sys.Date()

Details

DETAILS

Value

None; writes summary reports to file

See Also

[read_xlsx][readxl::read_xlsx] [mutate][dplyr::mutate], [filter][dplyr::filter], [select][dplyr::select], [distinct][dplyr::distinct], [left_join][dplyr::left_join], [pull][dplyr::pull], [ensym][dplyr::ensym] [replace_na][tidyr::replace_na] [tibble][tibble::tibble] [write.xlsx][openxlsx::write.xlsx]

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

%>%

%>%

Pipe operator

Description

See magrittr::%>% for details.

Usage

1hs %>% rhs

Arguments

1hs A value or the magrittr placeholder.

rhs A function call using the magrittr semantics.

Value

The result of calling 'rhs(lhs)'.

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