Package 'toxEval'

October 9, 2020

Type Package

Title Exploring Biological Relevance of Environmental Chemistry
Observations

Version 1.2.0

Description Data analysis package for estimating potential biological effects from chemical concentrations in environmental samples. Included are a set of functions to analyze, visualize, and organize measured concentration data as it relates to user-selected chemical-biological interaction benchmark data such as water quality criteria. The intent of these analyses is to develop a better understanding of the potential biological relevance of environmental chemistry data. Results can be used to prioritize which chemicals at which sites may be of greatest concern. These methods are meant to be used as a screening technique to predict potential for biological influence from chemicals that ultimately need to be validated with direct biological assays. A description of the analysis can be found in Blackwell et al. (2017) <doi:10.1021/acs.est.7b01613>.

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https://www.usgs.gov/visual-id/credit_usgs.html#copyright

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toxEval-package   *Analyze ToxCast data in relation to measured concentrations.*

Description

toxEval includes a set of functions to analyze, visualize, and organize measured concentration data as it relates to ToxCast data (default) or other user-selected chemical-biological interaction benchmark data such as water quality criteria. The intent of these analyses is to develop a better understanding of the potential biological relevance of environmental chemistry data. Results can be used to prioritize which chemicals at which sites may be of greatest concern. These methods are meant to be used as a screening technique to predict potential for biological influence from chemicals that ultimately need to be validated with direct biological assays.

Details

Package:	toxEval
Type:	Package
License:	Unlimited for this package, dependencies have more restrictive licensing.
Copyright:	This software is in the public domain because it contains materials that originally came from the United States G
LazyLoad:	yes

Author(s)

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as.toxEval   *toxEval helper functions*

Description

A small collection of helper functions for toxEval

Usage

```
as.toxEval(x, ...)
```

Arguments

x	list or toxEval object
...	data frames to override data within the original x list.

Examples

```
path_to_tox <-  system.file("extdata", package="toxEval")
file_name <- "OWC_data_fromSup.xlsx"
full_path <- file.path(path_to_tox, file_name)
tox_list <- create_toxEval(full_path)

# To over-ride one of the data frames:
chem_data <- data.frame(CAS = "21145-77-7",
                        Value = 1,
                        "Sample Date" = as.Date("2012-01-01"),
                        SiteID = "USGS-04249000")
tox_list_new <- as.toxEval(tox_list, chem_data)
```

---

clean_endPoint_info   *clean_endPoint_info*

Description

Define a subset of the ToxCast database for relevance to toxEval analyses. Subsetting is done based
upon methods defined by Blackwell et al., 2017. Specifically, this function removes endPoints
that are ATG sources with signal loss, and NVS with signal gain (basically: some assay/signal
combinations are removed because they target non-specific endpoints). Also, this function adds
additional categories to intended_target_family and intended_target_family_sub as described in the
paper linked above.

Usage

```
clean_endPoint_info(end_point_info)
```

Arguments

end_point_info   Data frame Endpoint information from ToxCast.

Value

The returned data frame is based on end_point_info, but with some endPoints filtered out and some
additional categories in intended_target_family and intended_target_family_sub. The names in in-
tended_target_family are revised to look more appealing in graphs and tables.

Examples

```
end_point_info <- end_point_info
nrow(end_point_info)
cleaned_ep <- clean_endPoint_info(end_point_info)
nrow(cleaned_ep)
```

| create_toxEval | *Load and check toxEval data* |

Description

This function is used to load a data file for analysis in the form of a single Excel file. The Excel file should include 3 mandatory sheets named "Data", "Chemicals", and "Sites". Additionally there are 2 optional sheets: "Exclude" and "Benchmarks". This function creates a data frame for each sheet, perform basic checks on the data to assure that required columns are included for each sheet

Usage

```
create_toxEval(excel_file_path, ...)
```

Arguments

excel_file_path

Path to Excel file that contains at least 3 sheets: Data, Chemicals, and Sites, and could optionally contain Exclude and Benchmarks.

...   data frames to override data within the original x list.

Details

Required columns in the Data sheet include "CAS", "SiteID", "Value", and "Sample Date". The "Value" column includes concentration measurements in units of μg/L. "Sample Date" can be either a date or date/time or an integer. Additional columns may be included for user purposes, but will not be used in toxEval.

Required columns in the Chemical sheet include "CAS", "Class". "CAS" values in this sheet must exactly match corresponding "CAS" values in the Data sheet. The "Class" designation allows data to be grouped in a user-specified way. For example, in a data set of multiple pesticides, it may be valuable to explore differences and similarities to of insecticides, herbicides and fungicides. Additional columns may be included for user purposes, but will not be used in toxEval.

Required columns in the Sites sheet includes "SiteID", "Short Name", and for the Shiny application "dec_lat","dec_lon". Values in the "SiteID" column in this sheet exactly match corresponding values in the "SiteID" column in the Data sheet. Additional columns may be included for user purposes, but will not be used in toxEval.

When using the optional sheet Exclude, columns required include "CAS" and "endPoint". These are used to exclude particular chemicals (via CAS), ToxCast endpoints (via endPoint), or a unique chemical/endpoint combination. Additional columns may be included for user purposes, but will not be used in toxEval.

When using the optional sheet Benchmarks, columns required include "CAS", "endPoint","ACC_value" and "chnm". This sheet is used to over-ride the functions using endpoints from the ToxCast database, allowing the user to import endpoint information from other sources. It could also be useful for reproducing results in the future (for example, if after ToxCast updates, analysis with an older version of ToxCast may be reproduced by including the selected ToxCast endpoint database in this sheet. Additional columns may be included for user purposes, but will not be used in toxEval.

For more information, see the "Prepare Data" vignette: `vignette("PrepareData", package = "toxEval")`.

All remaining toxEval functions use data from via the list that is returned from this function.

Value

The object returned from this function contains a list of between three and five data frames. The minimum data frames returned are chem_data (containing at least the columns: "CAS", "SiteID", "Value", "Sample Date"), chem_info (containing at least the columns: "CAS", "Class"), and chem_site (containing at least the columns: "SiteID", "Short Name". For the Shiny app, "dec_lat" and "dec_lon" are also required). The optional data frames are exclusions (containing at least the columns: "CAS" and "endPoint"), and benchmarks (containing at least the columns: "CAS", "end-Point", "ACC_value" and "chnm")

Examples

```
path_to_tox <-  system.file("extdata", package="toxEval")
file_name <- "OWC_data_fromSup.xlsx"
excel_file_path <- file.path(path_to_tox, file_name)
tox_list <- create_toxEval(excel_file_path)
```

---

endpoint_hits_DT   *Rank endpoints by category*

Description

The `endpoint_hits_DT` (data.table (DT) option) and `endpoint_hits` (data frame option) functions create tables with one row per endPoint, and one column per category("Biological", "Chemical", or "Chemical Class"). The values in the table are the number of sites where the EAR exceeded the user-defined EAR hit_threshold in that endpoint/category combination. If the category "Chemical" is chosen, an "info" link is provided to the chemical information available in the "Comptox Dashboard" https://comptox.epa.gov/dashboard/.

Usage

```
endpoint_hits_DT(
  chemical_summary,
  category = "Biological",
  mean_logic = FALSE,
  sum_logic = TRUE,
  hit_threshold = 0.1,
  include_links = TRUE
)

endpoint_hits(
  chemical_summary,
  category = "Biological",
```

```
    mean_logic = FALSE,
    sum_logic = TRUE,
    hit_threshold = 0.1
)
```

Arguments

chemical_summary
: Data frame from `get_chemical_summary`

category
: Character. Either "Biological", "Chemical Class", or "Chemical".

mean_logic
: Logical. `TRUE` displays the mean sample from each site, `FALSE` displays the maximum sample from each site.

sum_logic
: Logical. `TRUE` sums the EARs in a specified grouping, `FALSE` does not. `FALSE` indicates that EAR values are not considered to be additive and often will be a more appropriate choice for traditional benchmarks as opposed to ToxCast benchmarks.

hit_threshold
: Numeric. EAR threshold defining a "hit".

include_links
: Logical. whether or not to include a link to the ToxCast dashboard. Only needed for the "Chemical" category.

Details

The tables show slightly different results when choosing to explore data from a single site rather than all sites. The value displayed in this instance is the number of samples with hits rather than the number of sites with hits.

Value

data frame with one row per endpoint that had a hit (based on the hit_threshold). The columns are based on the category.

Examples

```
# This is the example workflow:
path_to_tox <-  system.file("extdata", package="toxEval")
file_name <- "OWC_data_fromSup.xlsx"

full_path <- file.path(path_to_tox, file_name)

tox_list <- create_toxEval(full_path)

ACC <- get_ACC(tox_list$chem_info$CAS)
ACC <- remove_flags(ACC)

cleaned_ep <- clean_endPoint_info(end_point_info)
filtered_ep <- filter_groups(cleaned_ep)
chemical_summary <- get_chemical_summary(tox_list, ACC, filtered_ep)

hits_df <- endpoint_hits(chemical_summary, category = "Biological")
```

```
endpoint_hits_DT(chemical_summary, category = "Biological")
endpoint_hits_DT(chemical_summary, category = "Chemical Class")
endpoint_hits_DT(chemical_summary, category = "Chemical")
```

---

end_point_info   *Endpoint information from ToxCast*

Description

Downloaded on October 2018 from ToxCast. The file name of the raw data was "Assay_Summary_190226.csv" from the zip file "INVITRODB_V3_1_SUMMARY" folder. At the time of the toxEval package release, these data were found at: <https://www.epa.gov/chemical-research/exploring-toxcast-data-downloadable-> in the section marked "Download Assay Information", in the ToxCast & Tox21 high-throughput assay information data set.

Value

data frame with 86 columns. The columns and definitions are discussed in the "ToxCast Assay Annotation Version 1.0 Data User Guide (PDF)" (see source)

Source

<https://doi.org/10.23645/epacomptox.6062479.v3>

References

U.S. EPA. 2014. ToxCast Assay Annotation Data User Guide. https://www.epa.gov/chemical-research/toxcast-assay-annotation-data-user-guide.

Examples

```
end_point_info <- end_point_info
head(end_point_info[,1:5])
```

---

explore_endpoints   *Explore data in the Shiny Application*

Description

Open an interactive app in a browser. See the "Shiny App" vignette: vignette("shinyApp", package = "toxEval") for more details. Using this function is a quick and convenient way to explore data. For more customization, the R-code to produce each graph and table is displayed in the app. That is a good starting-point for a custom analysis.

Usage

```
explore_endpoints(browse = TRUE)
```

Arguments

browse	Logical. Use browser for running Shiny app.

---

filter_groups	*Filter endPoints based on groups and assays.*

Description

This function provides a mechanism to specify 3 levels of information in the supplied data frame end_point_info to be used in subsequent analysis steps. First, the user specifies the ToxCast assay annotation using the 'groupCol' argument, which is a column header in 'end_point_info'. Second, the user specifies the families of assays to use. Finally, the user can choose to remove specific group(s) from the category. The default is to remove 'Background Measurement' and 'Undefined'. Choices for this should be reconsidered based on individual study objectives.

Usage

```
filter_groups(
  ep,
  groupCol = "intended_target_family",
 assays = c("ACEA", "APR", "ATG", "NVS", "OT", "TOX21", "CEETOX", "CLD", "TANGUAY",
   "NHEERL_PADILLA", "NCCT", "NHEERL_HUNTER", "NHEERL_NIS", "NHEERL_MED", "UPITT"),
  remove_groups = c("Background Measurement", "Undefined")
)
```

Arguments

ep	Data frame containing Endpoint information from ToxCast
groupCol	Character name of ToxCast annotation column to use as a group catetory
assays	Vector of assays to use in the data analysis. Possible values are "ACEA", "APR", "ATG", "BSK", "NVS", "OT", "TOX21", "CEETOX", "CLD", "TANGUAY", "NHEERL_PADILLA", "NCCT", "NHEERL_HUNTER", "NHEERL_NIS", "NHEERL_MED", "UPITT". By default, the "BSK" (BioSeek) assay is removed.
remove_groups	Vector of groups within the selected 'groupCol' to remove.

Details

The default category ('groupCol') is 'intended_target_family'. Depending on the study, other categories may be more relevant. The best resource on these groupings is the "ToxCast Assay Annotation Data User Guide" directly from EPA https://www.epa.gov/chemical-research/toxcast-assay-annotation-data-user-guide. Following that link, it defines "intended_target_family" as "the target family of the objective target for the assay". Much more detail can be discovered in that documentation.

Examples

```
end_point_info <- end_point_info
cleaned_ep <- clean_endPoint_info(end_point_info)
filtered_ep <- filter_groups(cleaned_ep)
head(filtered_ep)
```

---

get_ACC   *Get the ACC values for a selection of chemicals*

Description

The get_ACC function retrieves the activity concentration at cutoff (ACC) values for specified chemicals.

Usage

```
get_ACC(CAS)
```

Arguments

CAS   Vector of CAS.

Details

The data used in toxEval were combined from files in the "INVITRODB_V3_LEVEL5" directory that were included in the October 2018 release of the ToxCast database. The function get_ACC will convert the ACC values in the ToxCast database from units of (log μM) to units of μg/L, and reformat the data as input to toxEval.

Value

data frame with columns CAS, chnm, flags, endPoint, ACC, MlWt, and ACC_value

Examples

```
CAS <- c("121-00-6","136-85-6","80-05-7","84-65-1","5436-43-1","126-73-8")
ACC <- get_ACC(CAS)
head(ACC)
```

---

get_chemical_summary   *Compute EAR values*

Description

This function computes Exposure:Activity ratios using user-provided measured concentration data from the output of create_toxEval, and joins the data with the activity concentration at cutoff data provided by ToxCast.Data from ToxCast is included with this package, but alternative benchmark data can be provided to perform the same "toxEval" analysis.

Usage

```
get_chemical_summary(
  tox_list,
  ACC = NULL,
  filtered_ep = "All",
  chem_data = NULL,
  chem_site = NULL,
  chem_info = NULL,
  exclusion = NULL
)
```

Arguments

tox_list	List with data frames for chem_data, chem_info, chem_site, and optionally exclusions and benchmarks. Created with create_toxEval.
ACC	Data frame with columns: CAS, chnm, endPoint, and ACC_value for specific chemical/endpoint combinations generated using the get_ACC function. End-Points with specific data quality flags may optionally be removed using the remove_flags function.
filtered_ep	Data frame with columns: endPoints, groupCol. Default is "All", where no filtering occurs.
chem_data	*Optional* data frame with (at least) columns: CAS, SiteID, and Value. Default is NULL. The argument will over-ride what is in tox_list.
chem_site	*Optional* data frame with (at least) columns: SiteID, and Short Name. Default is NULL. The argument will over-ride what is in tox_list.
chem_info	*Optional* data frame with (at least) columns: CAS, and class. Default is NULL. The argument will over-ride what is in tox_list.
exclusion	*Optional* data frame with (at least) columns: CAS and endPoint. Default is NULL. The argument will over-ride what is in tox_list.

Details

To use the data provided by the package, a sample workflow is shown below in the examples. The examples include retrieving the ToxCast (ACC) values that are used to calculate EARs, choosing endPoints that should be ignored based on data quality "flags" in the ToxCast database, and removing groups of endPoints that may not be important to the analysis at hand.

Value

a data frame with the columns: CAS, chnm (chemical name as a factor), site, date, EAR, Bio_category, shortName (of site), Class. The output of this function is where you find EAR values for every chemical/endpoint combination.

Examples

```
path_to_tox <-  system.file("extdata", package="toxEval")
file_name <- "OWC_data_fromSup.xlsx"
full_path <- file.path(path_to_tox, file_name)

tox_list <- create_toxEval(full_path)

ACC <- get_ACC(tox_list$chem_info$CAS)
ACC <- remove_flags(ACC)

cleaned_ep <- clean_endPoint_info(end_point_info)
filtered_ep <- filter_groups(cleaned_ep)

chemical_summary <- get_chemical_summary(tox_list, ACC, filtered_ep)
head(chemical_summary)
```

---

get_concentration_summary

Create concentration summary

Description

Use this function to create a chemical_summary, but instead of using any benchmarks, the EAR column is simply the concentration. The output of this function can be used in any of the plotting or table functions in the same way that the output of get_chemical_summary.

Usage

```
get_concentration_summary(
  tox_list,
  chem_data = NULL,
  chem_site = NULL,
  chem_info = NULL,
  tox_names = TRUE
)
```

Arguments

tox_list	List with data frames for chem_data, chem_info, and chem_site. Created with create_toxEval.
chem_data	*Optional* data frame with (at least) columns: CAS, SiteID, and Value. Default is NULL. The argument will over-ride what is in tox_list.

chem_site   *Optional* data frame with (at least) columns: SiteID, and Short Name. Default
               is NULL. The argument will over-ride what is in tox_list.

chem_info   *Optional* data frame with (at least) columns: CAS, and class. Default is NULL.
               The argument will over-ride what is in tox_list.

tox_names   Logical whether to use the provided chemical names from the ToxCast or not.
               If there is not a match by CAS, the function will look for a column "Chemical"
               in the "Chemical" tab. If that column doesn't exist, it will create a (not good!)
               name.

Value

a data frame with the columns: CAS, chnm (chemical name as a factor), site, date, EAR (which is
just concentration), Bio_category, shortName (of site), Class. The output of this function is where
you find EAR values for every chemical/endpoint combination.

Examples

```
path_to_tox <-  system.file("extdata", package="toxEval")
file_name <- "OWC_data_fromSup.xlsx"
full_path <- file.path(path_to_tox, file_name)

tox_list <- create_toxEval(full_path)

chemical_summary_conc <- get_concentration_summary(tox_list)
head(chemical_summary_conc)
plot_tox_boxplots(chemical_summary_conc,
                  category = "Chemical",
                  x_label = "Concentration [ug/L]")
```

---

graph_chem_data   *Prepare boxplot data*

Description

A set of functions to prepare the data for boxplots. Often, these functions are used within the
plotting functions. They are exported however to allow custom graphs to be created.

Usage

```
graph_chem_data(
  chemical_summary,
  ...,
  manual_remove = NULL,
  mean_logic = FALSE,
  sum_logic = TRUE
)

tox_boxplot_data(
```

```
  chemical_summary,
  category = "Biological",
  manual_remove = NULL,
  mean_logic = FALSE,
  sum_logic = TRUE
)

side_by_side_data(
  gd_left,
  gd_right,
  left_title = "Left",
  right_title = "Right"
)
```

Arguments

chemical_summary
> Data frame from [get_chemical_summary](#).

...   Additional group_by arguments. This can be handy for creating facet graphs.

manual_remove   Vector of categories to remove.

mean_logic   Logical. TRUE displays the mean sample from each site, FALSE displays the maximum sample from each site.

sum_logic   Logical. TRUE sums the EARs in a specified grouping, FALSE does not. FALSE may be better for traditional benchmarks as opposed to ToxCast benchmarks.

category   Character. Either "Biological", "Chemical Class", or "Chemical".

gd_left   Data frame that must include the columns chnm, Class, and either EAR or mean-EAR.

gd_right   Data frame that must include the columns chnm, Class, and either EAR or mean-EAR.

left_title   Character that will be associated with the "gd_left" data frame in a column named "guide_side".

right_title   Character that will be associated with the "gd_right" data frame in a column named "guide_side".

Details

The function side_by_side_data will combine two data frames, either the output of [get_chemical_summary](#) or [graph_chem_data](#), into a single data frame. The important work here is that the chemicals and classes factor levels are ordered primarily based on "gd_left", but include "gd_right" when the contents are mismatched.

Examples

```
path_to_tox <-  system.file("extdata", package="toxEval")
file_name <- "OWC_data_fromSup.xlsx"
full_path <- file.path(path_to_tox, file_name)
```

```
tox_list <- create_toxEval(full_path)

ACC <- get_ACC(tox_list$chem_info$CAS)
ACC <- remove_flags(ACC)

cleaned_ep <- clean_endPoint_info(end_point_info)
filtered_ep <- filter_groups(cleaned_ep)

chemical_summary <- get_chemical_summary(tox_list, ACC, filtered_ep)
# Let's say we want to compare 2 chemical summaries
# We'll look at one summing EARs, and with concentrations
# First, we need a chemical summary for concentrations:
chemical_summary_conc <- get_concentration_summary(tox_list)

gd_tox <- graph_chem_data(chemical_summary)
gd_conc <- graph_chem_data(chemical_summary_conc)

ch_combo <- side_by_side_data(gd_tox, gd_conc,
                              left_title = "ToxCast",
                              right_title = "Concentrations")
plot_chemical_boxplots(ch_combo, guide_side,
                       x_label = "") +
  ggplot2::facet_grid(. ~ guide_side, scales = "free_x")
```

---

hits_by_groupings_DT   *Biological hits per category*

Description

The `hits_by_groupings_DT` (DT option) and `hits_by_groupings` (data frame option) functions create tables with one row per category("Biological", "Chemical", or "Chemical Class"). The columns indicate the "Biological" groupings. The values in the table signify how many sites have samples with EARs that exceeded the hit_threshold for that particular "Biological"/category combination. If the user chooses "Biological" as the category, it is a simple 2-column table of "Biological" groupings and number of sites (nSites).

Usage

```
hits_by_groupings_DT(
  chemical_summary,
  category = "Biological",
  mean_logic = FALSE,
  sum_logic = TRUE,
  hit_threshold = 0.1
)

hits_by_groupings(
  chemical_summary,
  category,
```

```
  mean_logic = FALSE,
  sum_logic = TRUE,
  hit_threshold = 0.1
)
```

Arguments

chemical_summary

                 Data frame from [get_chemical_summary](#).

category   Character. Either "Biological", "Chemical Class", or "Chemical".

mean_logic   Logical. TRUE displays the mean sample from each site, FALSE displays the maximum sample from each site.

sum_logic   Logical. TRUE sums the EARs in a specified grouping, FALSE does not. FALSE may be better for traditional benchmarks as opposed to ToxCast benchmarks.

hit_threshold   Numeric threshold defining a "hit".

Details

The tables result in slightly different results for a single site, displaying the number of samples with hits rather than the number of sites.

Value

data frame with one row per category, and one column per Biological grouping.

Examples

```
# This is the example workflow:
path_to_tox <-  system.file("extdata", package="toxEval")
file_name <- "OWC_data_fromSup.xlsx"

full_path <- file.path(path_to_tox, file_name)

tox_list <- create_toxEval(full_path)

ACC <- get_ACC(tox_list$chem_info$CAS)
ACC <- remove_flags(ACC)

cleaned_ep <- clean_endPoint_info(end_point_info)
filtered_ep <- filter_groups(cleaned_ep)
chemical_summary <- get_chemical_summary(tox_list, ACC, filtered_ep)

site_df <- hits_by_groupings(chemical_summary, category = "Biological")

hits_by_groupings_DT(chemical_summary, category = "Biological")
hits_by_groupings_DT(chemical_summary, category = "Chemical Class")
hits_by_groupings_DT(chemical_summary, category = "Chemical")
```

---

hits_summary_DT   *Summary of hits per site/category*

Description

The hits_summary_DT (DT option) and hits_summary (data frame option) functions create tables
information on the number of hit_threshold exceedances per site for each individual grouping.
The table has one row per group per site that has hit_threshold exceedances. For example, if
"Biological" is the category, and a site has EAR levels above the specified hit_threshold for
"DNA Binding" and "Nuclear Receptors", that site will have 2 rows of data in this table.

Usage

```
hits_summary_DT(
  chemical_summary,
  category = "Biological",
  sum_logic = TRUE,
  hit_threshold = 0.1
)

hits_summary(chemical_summary, category, hit_threshold = 0.1, sum_logic = TRUE)
```

Arguments

chemical_summary

Data frame from [get_chemical_summary](#).

category   Character. Either "Biological", "Chemical Class", or "Chemical".

sum_logic   Logical. TRUE sums the EARs in a specified grouping, FALSE does not. FALSE
                  may be better for traditional benchmarks as opposed to ToxCast benchmarks.

hit_threshold   Numeric threshold defining a "hit".

Details

For each row, there are 4 columns. Site and category (as defined by the category argument) define
the row. "Samples with hits" are how many samples exceeded the hit_threshold for the specified
category at the specified site. "Number of Samples" indicates how many samples were collected at
an individual site based on unique date.

The tables contain slightly different results for evaluation of a single site. There are three columns
(the Site column is dropped), and rather than one row per site/category, there is one row per category.

Value

data frame with with one row per unique site/category combination. The columns are site, category,
Samples with Hits, and Number of Samples.

data frame with columns "Hits per Sample", "Individual Hits", "nSample", "site", and "category"

Examples

```
# This is the example workflow:
path_to_tox <-  system.file("extdata", package="toxEval")
file_name <- "OWC_data_fromSup.xlsx"

full_path <- file.path(path_to_tox, file_name)

tox_list <- create_toxEval(full_path)

ACC <- get_ACC(tox_list$chem_info$CAS)
ACC <- remove_flags(ACC)

cleaned_ep <- clean_endPoint_info(end_point_info)
filtered_ep <- filter_groups(cleaned_ep)
chemical_summary <- get_chemical_summary(tox_list, ACC, filtered_ep)

stats_group <- hits_summary(chemical_summary, "Biological")

hits_summary_DT(chemical_summary, category = "Biological")
hits_summary_DT(chemical_summary, category = "Chemical Class")
hits_summary_DT(chemical_summary, category = "Chemical")
```

---

make_tox_map   *Create an interactive map of the data*

Description

The function make_tox_map creates a leaflet map of the sites. This function places symbols at
the location of each site in the data file that represent the magnitude of EAR (color) and the number
of samples in the data set (size). This is the only function that requires "dec_lon" and "dec_lat"
(decimal longitude and decimal latitude) in the data frame specified for the chem_site argument.

Usage

```
make_tox_map(
  chemical_summary,
  chem_site,
  category = "Biological",
  mean_logic = FALSE,
  sum_logic = TRUE
)

map_tox_data(
  chemical_summary,
  chem_site,
  category = "Biological",
  mean_logic = FALSE,
```

```
    sum_logic = TRUE
)
```

Arguments

chemical_summary

> Data frame from [get_chemical_summary](#).

chem_site
> Data frame containing the columns SiteID, site_grouping, Short Name, dec_lon, and dec_lat.

category
> Character. Either "Biological", "Chemical Class", or "Chemical".

mean_logic
> Logical. TRUE displays the mean EAR from each site, FALSE displays the maximum EAR from each site.

sum_logic
> Logical. TRUE sums the EARs in a specified grouping, FALSE does not. FALSE may be better for traditional benchmarks as opposed to ToxCast benchmarks.

Details

The function map_tox_data calculates the statistics for the map. It my be useful on it's own.

Examples

```
# This is the example workflow:
path_to_tox <-  system.file("extdata", package="toxEval")
file_name <- "OWC_data_fromSup.xlsx"

full_path <- file.path(path_to_tox, file_name)
tox_list <- create_toxEval(full_path)

ACC <- get_ACC(tox_list$chem_info$CAS)
ACC <- remove_flags(ACC)

cleaned_ep <- clean_endPoint_info(end_point_info)
filtered_ep <- filter_groups(cleaned_ep)
chemical_summary <- get_chemical_summary(tox_list, ACC, filtered_ep)

make_tox_map(chemical_summary, tox_list$chem_site, "Biological")
make_tox_map(chemical_summary, tox_list$chem_site, "Chemical Class")
make_tox_map(chemical_summary, tox_list$chem_site, "Chemical")
```

---

plot_chemical_boxplots

Grouped Boxplots

Description

The `plot_tox_boxplots` function creates a set of boxplots representing EAR values computed
with the [get_chemical_summary](#) function, and dependent on the choice of several input options.
See "Summarizing the data" in the Introduction vignette: `vignette("Introduction", package`
`= "toxEval").` for a description of how the EAR values are computed, aggregated, and summa-
rized. Choosing "Chemical Class" in the category argument will generate separate boxplots for
each unique class. "Chemical" will generate boxplots for each individual chemical, and "Biologi-
cal" will generate boxplots for each group in the selected ToxCast annotation.

Usage

```
plot_chemical_boxplots(
  chemical_summary,
  ...,
  manual_remove = NULL,
  mean_logic = FALSE,
  sum_logic = TRUE,
  plot_ND = TRUE,
  font_size = NA,
  title = NA,
  x_label = NA,
  palette = NA,
  hit_threshold = NA
)

plot_tox_boxplots(
  chemical_summary,
  category = "Biological",
  manual_remove = NULL,
  mean_logic = FALSE,
  sum_logic = TRUE,
  plot_ND = TRUE,
  font_size = NA,
  title = NA,
  x_label = NA,
  palette = NA,
  hit_threshold = NA
)
```

Arguments

chemical_summary
                   Data frame from [get_chemical_summary](#).

...   Additional group_by arguments. This can be handy for creating facet graphs.

manual_remove   Vector of categories to remove.

mean_logic   Logical. `TRUE` displays the mean sample from each site, `FALSE` displays the
                   maximum sample from each site.

sum_logic	Logical. TRUE sums the EARs in a specified grouping, FALSE does not. FALSE may be better for traditional benchmarks as opposed to ToxCast benchmarks.
plot_ND	Logical. Whether or not to plot "Biological" groupings, "Chemical Class" groupings, or "Chemical" that do not have any detections.
font_size	Numeric value to adjust the axis font size.
title	Character title for plot. Default is NA which produces no title.
x_label	Character for x label. Default is NA which produces an automatic label.
palette	Vector of color palette for boxplot fill. Can be a named vector to specify specific colors for specific categories.
hit_threshold	Numeric threshold defining a "hit".
category	Character. Either "Biological", "Chemical Class", or "Chemical".

Details

It is also possible to display a threshold line using the hit_threshold argument. The graph will then include the number of sites with detections, the threshold line, and the number of "hits" indicating how many sites that have EAR values exceeding the hit_threshold.

The graph shows a slightly different result for a single site. For a single site graph, the number of chemicals that were detected and have associated endpoint ACCs represented are displayed.

The functions plot_tox_boxplots and graph_chem_data are functions that perform the statistical calculations to create the plot. graph_chem_data is specific to the "Chemical" plot, and plot_tox_boxplots is for "Biological" and "Chemical Class".

Box plots are standard Tukey representations. See "Box plot details" in the Basic Workflow vignette: vignette("basicWorkflow", package = "toxEval") for more information.

Examples

```
# This is the example workflow:
path_to_tox <-  system.file("extdata", package="toxEval")
file_name <- "OWC_data_fromSup.xlsx"

full_path <- file.path(path_to_tox, file_name)

tox_list <- create_toxEval(full_path)
ACC <- get_ACC(tox_list$chem_info$CAS)
ACC <- remove_flags(ACC)

cleaned_ep <- clean_endPoint_info(end_point_info)
filtered_ep <- filter_groups(cleaned_ep)
chemical_summary <- get_chemical_summary(tox_list, ACC, filtered_ep)
plot_tox_boxplots(chemical_summary, "Biological")
plot_tox_boxplots(chemical_summary, "Chemical Class")
plot_tox_boxplots(chemical_summary, "Chemical")


cbPalette <- c("#999999", "#E69F00", "#56B4E9", "#009E73", "#F0E442",
               "#0072B2", "#D55E00", "#CC79A7")
graphData <- tox_boxplot_data(chemical_summary = chemical_summary,
```

```
                                        category = "Biological")
cbValues <- colorRampPalette(cbPalette)(length(levels(graphData$category)))
names(cbValues) <- levels(graphData$category)

plot_tox_boxplots(chemical_summary,
                  hit_threshold = 0.1,
                  category = "Biological",
                  palette = cbValues,
                title = 'Maximum EAR per site, grouped by biological activity groupings')

plot_tox_boxplots(chemical_summary,
                  category = "Chemical", x_label = "EAR")
single_site <- dplyr::filter(chemical_summary, site == "USGS-04024000")
plot_tox_boxplots(single_site,
                  category = "Biological")
plot_tox_boxplots(single_site,
                  category = "Chemical", hit_threshold = 0.001)
```

---

plot_tox_endpoints   *EndPoint boxplots*

Description

The `plot_tox_endpoints` function creates a set of boxplots representing EAR values for each endPoint based on the selected data. A subset of data is first chosen by specifying a group in the filterBy argument. The filterBy argument must match one of the unique options in the category. For example, if the category is "Chemical Class", then the filterBy argument must be one of the defined "Chemical Class" options such as "Herbicide". A boxplot is generated for each endPoint. The EAR values that are used to create the boxplots are the mean or maximum (as defined by mean_logic) for each site as described in "Summarizing the data"in the Introduction vignette: `vignette("Introduction", package = "toxEval")`.

Usage

```
plot_tox_endpoints(
  chemical_summary,
  category = "Biological",
  filterBy = "All",
  manual_remove = NULL,
  hit_threshold = NA,
  mean_logic = FALSE,
  sum_logic = TRUE,
  font_size = NA,
  title = NA,
  x_label = NA,
  palette = NA,
  top_num = NA
)
```

Arguments

`chemical_summary`	Data frame from [`get_chemical_summary`](#).
`category`	Either "Biological", "Chemical Class", or "Chemical".
`filterBy`	Character. Either "All" or one of the filtered categories.
`manual_remove`	Vector of categories to remove.
`hit_threshold`	Numeric threshold defining a "hit".
`mean_logic`	Logical. TRUE displays the mean sample from each site, FALSE displays the maximum sample from each site.
`sum_logic`	logical. TRUE sums the EARs in a specified grouping, FALSE does not. FALSE may be better for traditional benchmarks as opposed to ToxCast benchmarks.
`font_size`	Numeric to adjust the axis font size.
`title`	Character title for plot.
`x_label`	Character for x label. Default is NA which produces an automatic label.
`palette`	Vector of color palette for fill. Can be a named vector to specify specific color for specific categories.
`top_num`	Integer number of endpoints to include in the graph. If NA, all endpoints will be included.

Details

Box plots are standard Tukey representations. See "Box plot details" in the Basic Workflow vignette: `vignette("basicWorkflow", package = "toxEval")` for more information.

Examples

```
# This is the example workflow:
path_to_tox <-  system.file("extdata", package="toxEval")
file_name <- "OWC_data_fromSup.xlsx"

full_path <- file.path(path_to_tox, file_name)

tox_list <- create_toxEval(full_path)
ACC <- get_ACC(tox_list$chem_info$CAS)
ACC <- remove_flags(ACC)

cleaned_ep <- clean_endPoint_info(end_point_info)
filtered_ep <- filter_groups(cleaned_ep)
chemical_summary <- get_chemical_summary(tox_list, ACC, filtered_ep)

plot_tox_endpoints(chemical_summary,
                   filterBy = "Cell Cycle",
                   top_num = 10)
plot_tox_endpoints(chemical_summary,
                   filterBy = "Cell Cycle",
                   top_num = 10,
                   x_label = "EAR")
```

```
plot_tox_endpoints(chemical_summary,
                     category = "Chemical Class", filterBy = "PAHs",
                     top_num = 10, hit_threshold = 0.001)
plot_tox_endpoints(chemical_summary, category = "Chemical", filterBy = "Atrazine")
plot_tox_endpoints(chemical_summary, category = "Chemical", top_num = 10)
single_site <- dplyr::filter(chemical_summary, site == "USGS-04024000")
plot_tox_endpoints(single_site, category = "Chemical", top_num = 10)
```

---

plot_tox_heatmap   *Plot EAR heat maps*

Description

The `plot_tox_heatmap` function creates a heat (tile) map with sites on the x-axis, a specified group-
ing on the y-axis (defined by the category argument), and color shading defining the mean or maxi-
mum EAR. See "Summarizing the data" in the Introduction vignette: vignette("Introduction",
package = "toxEval") for a description on how the EAR values are computed, aggregated, and
summarized. The y-axis grouping can be "Biological", "Chemical Class", or "Chemical". When
specifying the "Chemical" option, a secondary y-axis is automatically included to group chemicals
into chemical class. The function computes default breaks for the color scale to match the spread
of the data, but breaks can also be customized with the breaks argument. This is a function where it
may be ideal to create a custom order to the sites (for example, west-to-east). See the above section
"Custom configuration" vignette("Introduction", package = "toxEval") for instructions on
how to convert the character vector sites to a factor with ordered levels.

Usage

```
plot_tox_heatmap(
  chemical_summary,
  chem_site,
  category = "Biological",
  breaks = c(1e-05, 1e-04, 0.001, 0.01, 0.1, 1, 10),
  manual_remove = NULL,
  mean_logic = FALSE,
  sum_logic = TRUE,
  plot_ND = TRUE,
  font_size = NA,
  title = NA,
  legend_lab = NA
)
```

Arguments

chemical_summary

       Data frame from `get_chemical_summary`.

chem_site   Data frame with columns SiteID, site_grouping, and Short Name.

category   Either "Biological", "Chemical Class", or "Chemical".

breaks	Numerical vector to define data bins and legend breaks.
manual_remove	Vector of categories to remove.
mean_logic	Logical. TRUE displays the mean sample from each site, FALSE displays the maximum sample from each site.
sum_logic	Logical. TRUE sums the EARs in a specified grouping, FALSE does not. FALSE may be better for traditional benchmarks as opposed to ToxCast benchmarks.
plot_ND	Logical. Whether or not to plot "Biological" groupings, "Chemical Class" groupings, or "Chemical" that do not have any detections.
font_size	Numeric value to adjust the axis font size.
title	Character title for plot.
legend_lab	Character label for legend. Default is NA which produces an automatic label.

Details

If there are site/parameters (chemical/chemical class/biological grouping) combinations that don't have data, those areas are represented by an "X". If there are 0 values, they are considered "non-detects", and represented with a distinct color.

Examples

```
path_to_tox <- system.file("extdata", package="toxEval")
file_name <- "OWC_data_fromSup.xlsx"
full_path <- file.path(path_to_tox, file_name)

tox_list <- create_toxEval(full_path)

ACC <- get_ACC(tox_list$chem_info$CAS)
ACC <- remove_flags(ACC)

cleaned_ep <- clean_endPoint_info(end_point_info)
filtered_ep <- filter_groups(cleaned_ep)

chemical_summary <- get_chemical_summary(tox_list, ACC, filtered_ep)

#Order the site_groupings:
tox_list$chem_site$site_grouping <- factor(tox_list$chem_site$site_grouping,
            levels=c("Lake Superior",
            "Lake Michigan",
            "Lake Huron",
            "Lake Erie",
            "Lake Ontario"))

#Order sites:
sitesOrdered <- c("StLouis","Nemadji","WhiteWI","Bad","Montreal",
"PresqueIsle","Ontonagon","Sturgeon","Tahquamenon","Burns",
"IndianaHC","StJoseph","PawPaw","Kalamazoo","GrandMI",
"Milwaukee","Muskegon","WhiteMI","PereMarquette","Manitowoc",
"Manistee","Fox","Oconto","Peshtigo","Menominee",
"Indian","Cheboygan","Ford","Escanaba","Manistique",
```

```
"ThunderBay","AuSable","Rifle","Saginaw","BlackMI",
"Clinton","Rouge","HuronMI","Raisin","Maumee",
"Portage","Sandusky","HuronOH","Vermilion","BlackOH",
"Rocky","Cuyahoga","GrandOH","Cattaraugus","Tonawanda",
"Genesee","Oswego","BlackNY","Oswegatchie","Grass",
"Raquette","StRegis")

tox_list$chem_site$`Short Name` <- factor(tox_list$chem_site$`Short Name`,
              levels = sitesOrdered)
plot_tox_heatmap(chemical_summary, tox_list$chem_site, category = "Chemical Class")
plot_tox_heatmap(chemical_summary, tox_list$chem_site,
                 category = "Chemical", legend_lab = "EAR")

single_site <- dplyr::filter(chemical_summary, site == "USGS-04024000")
plot_tox_heatmap(chemical_summary = single_site,
               chem_site = dplyr::filter(tox_list$chem_site, SiteID == "USGS-04024000"),
               category = "Chemical Class")
plot_tox_heatmap(chemical_summary = single_site,
               chem_site = dplyr::filter(tox_list$chem_site, SiteID == "USGS-04024000"),
               category = "Chemical")
```

---

plot_tox_stacks   *Plot stacked bar charts*

Description

The `plot_tox_stacks` function creates a set of boxplots representing EAR values computed with
the [get_chemical_summary](#) function, and dependent on the choice of several input options. See
"Summarizing the data" in the Introduction vignette: [vignette("Introduction", package = "toxEval")](#)
for a description on how the EAR values are computed, aggregated, and summarized. Choosing
"Chemical Class" in the category argument will generate separate stacked bars for each unique
class. "Chemical" will generate stacked bars for each individual chemical, and "Biological" will
generate stacked bars for each group in the selected ToxCast annotation. The legend can optionally
be turned on or off using the include_legend argument. It may be impractical for instance to show
the legend for "Chemical" if there are hundreds of chemicals.

Usage

```
plot_tox_stacks(
  chemical_summary,
  chem_site,
  category = "Biological",
  mean_logic = FALSE,
  sum_logic = TRUE,
  manual_remove = NULL,
  include_legend = TRUE,
  font_size = NA,
  title = NA,
  y_label = NA,
```

```
    top_num = NA
)
```

Arguments

chemical_summary

                   Data frame from `get_chemical_summary`.

chem_site   Data frame with at least columns SiteID, site_grouping, and Short Name.

category   Character. Either "Biological", "Chemical Class", or "Chemical".

mean_logic   Logical. TRUE displays the mean sample from each site, FALSE displays the maximum sample from each site.

sum_logic   Logical. TRUE sums the EARs in a specified grouping, FALSE does not. FALSE may be better for traditional benchmarks as opposed to ToxCast benchmarks.

manual_remove   Vector of categories to remove.

include_legend   Logical. Used to include legend or not.

font_size   Numeric value to adjust the axis font size.

title   Character title for plot.

y_label   Character for x label. Default is NA which produces an automatic label.

top_num   Integer number to include in the graph. If NA, all data will be included.

Details

The graph displays a slightly different result for a single site. Providing data with only one site displays each individual sample as a stacked bar rather than the mean or maximum for a site.

This is a function where it may be ideal to create a custom order to the sites (for example, west-to-east). See the above section "Custom configuration" `vignette("Introduction", package = "toxEval")` for instructions on how to convert the character vector sites to a factor with ordered levels.

Examples

```
# This is the example workflow:
path_to_tox <-  system.file("extdata", package="toxEval")
file_name <- "OWC_data_fromSup.xlsx"

full_path <- file.path(path_to_tox, file_name)

tox_list <- create_toxEval(full_path)

ACC <- get_ACC(tox_list$chem_info$CAS)
ACC <- remove_flags(ACC)

cleaned_ep <- clean_endPoint_info(end_point_info)
filtered_ep <- filter_groups(cleaned_ep)
chemical_summary <- get_chemical_summary(tox_list, ACC, filtered_ep)

plot_tox_stacks(chemical_summary, tox_list$chem_site, "Biological")
```

```
plot_tox_stacks(chemical_summary, tox_list$chem_site, "Chemical Class")
plot_tox_stacks(chemical_summary, tox_list$chem_site, "Chemical", include_legend = FALSE)
plot_tox_stacks(chemical_summary, tox_list$chem_site, "Chemical", top_num = 5, y_label = "EAR")

single_site <- dplyr::filter(chemical_summary, site == "USGS-04024000")
plot_tox_stacks(single_site, tox_list$chem_site, "Chemical", top_num = 5)
plot_tox_stacks(single_site, chem_site = tox_list$chem_site,
                category = "Chemical", top_num = 5, y_label = "EAR")
```

---

rank_sites_DT   *Rank sites by EAR*

Description

The `rank_sites_DT` (DT option) and `rank_sites` (data frame option) functions create tables with
one row per site. Columns represent the maximum or mean EAR (depending on the mean_logic
argument) for each category ("Chemical Class", "Chemical", or "Biological") and the frequency of
the maximum or mean EAR exceeding a user specified hit_threshold.

Usage

```
rank_sites_DT(
  chemical_summary,
  category = "Biological",
  mean_logic = FALSE,
  sum_logic = TRUE,
  hit_threshold = 0.1
)

rank_sites(
  chemical_summary,
  category,
  hit_threshold = 0.1,
  mean_logic = FALSE,
  sum_logic = TRUE
)
```

Arguments

chemical_summary
                 Data frame from [get_chemical_summary](#).

category   Character. Either "Biological", "Chemical Class", or "Chemical".

mean_logic   Logical. TRUE displays the mean sample from each site, FALSE displays the
                 maximum sample from each site.

sum_logic   Logical. TRUE sums the EARs in a specified grouping, FALSE does not. FALSE
                 may be better for traditional benchmarks as opposed to ToxCast benchmarks.

hit_threshold   Numeric threshold defining a "hit".

Details

The tables show slightly different results for a single site. Rather than multiple columns for categories, there is now 1 row per category (since the site is known).

Value

data frame with one row per site, and the mas or mean EAR and frequency of hits based on the category.

Examples

```
# This is the example workflow:
path_to_tox <-  system.file("extdata", package="toxEval")
file_name <- "OWC_data_fromSup.xlsx"

full_path <- file.path(path_to_tox, file_name)

tox_list <- create_toxEval(full_path)

ACC <- get_ACC(tox_list$chem_info$CAS)
ACC <- remove_flags(ACC)

cleaned_ep <- clean_endPoint_info(end_point_info)
filtered_ep <- filter_groups(cleaned_ep)
chemical_summary <- get_chemical_summary(tox_list, ACC, filtered_ep)

stats_df <- rank_sites(chemical_summary, "Biological")

rank_sites_DT(chemical_summary, category = "Biological")
rank_sites_DT(chemical_summary, category = "Chemical Class")
rank_sites_DT(chemical_summary, category = "Chemical")
```

---

remove_flags	*Remove endpoints with specific data quality flags from data*

Description

Through the ToxCast program quality assurance procedures, information is examined and at times, it is necessary to assign a data quality flag to a specific chemical/assay result. A toxEval user may want to include or exclude assay results with certain flags depending on the objectives of a given study. Assay results with specific data quality flags assigned to them can be removed based on their designated flag with the remove_flags function. The flags included in ToxCast, and the associated flagsShort value (used in the remove_flags function) are as follows:

Flag	flagsShort
Borderline active*	Borderline*
Only highest conc above baseline, active*	OnlyHighest*

Only one conc above baseline, active	OneAbove
Noisy data	Noisy
Hit-call potentially confounded by overfitting	HitCall
Gain AC50 < lowest conc & loss AC50 < mean conc*	GainAC50*
Biochemical assay with < 50% efficacy*	Biochemical*
Less than 50% efficacy	LessThan50
AC50 less than lowest concentration tested*	ACCLessThan*
GNLSmodel	GNLSmodel

Asterisks indicate flags removed in the function as default.

Usage

```
remove_flags(
  ACC,
  flagsShort = c("Borderline", "OnlyHighest", "GainAC50", "Biochemical", "ACCLessThan")
)
```

Arguments

ACC   data frame with columns: casn, chnm, endPoint, and ACC_value

flagsShort   vector of flags to to trigger REMOVAL of chemical:endPoint combination. Pos-
              sible values are "Borderline", "OnlyHighest", "OneAbove", "Noisy", "HitCall",
              "GainAC50", "Biochemical","LessThan50","ACCLessThan","GNLSmodel".

Examples

```
CAS <- c("121-00-6","136-85-6","80-05-7","84-65-1","5436-43-1","126-73-8")
ACC <- get_ACC(CAS)
nrow(ACC)
ACC <- remove_flags(ACC)
nrow(ACC)
```

---

summary.toxEval   *Summary of tox_list*

Description

A "tox_list" object is created from `create_toxEval`. It is a list of 5 data frames: chem_data,
chem_info, chem_site, exclusions, and benchmarks. This function returns a message with how
many chemicals have ToxCast information, and returns a vector of which chemicals do not have
ToxCast information.

Usage

```
## S3 method for class 'toxEval'
summary(object, ...)
```

Arguments

object   toxEval object with "chem_info" data frame included.

...   additional parameters

Examples

```
path_to_tox <-  system.file("extdata", package="toxEval")
file_name <- "OWC_data_fromSup.xlsx"
excel_file_path <- file.path(path_to_tox, file_name)
tox_list <- create_toxEval(excel_file_path)
summary(tox_list)
```

ToxCast_ACC   *ACC values included with toxEval.*

Description

Downloaded on January 2020 from ToxCast. The data were combined from files in the "INVIT-RODB_V3_LEVEL5" folder. At the time of toxEval package release, this information was found: <https://www.epa.gov/chemical-research/exploring-toxcast-data-downloadable-data> in the "ToxCast & Tox21 Data Spreadsheet" data set. ACC values are the in the "ACC" column (winning model) and units are log micro-Molarity (log μM).

Value

data frame with columns CAS, chnm (chemical name), flags, endPoint, and ACC (value).

Source

<https://www.epa.gov/chemical-research/exploring-toxcast-data-downloadable-data>

References

Toxicology, EPA's National Center for Computational (2018): ToxCast and Tox21 Data Spreadsheet. figshare. Dataset. https://doi.org/10.23645/epacomptox.6062503.v3

Examples

```
head(ToxCast_ACC)
```

---

tox_chemicals   *ToxCast Chemical Information*

Description

Downloaded on October 2015 from ToxCast. The file name of the raw data was "TOX21IDs_v4b_23Oct2014_QCdetails.xlsx" from the US EPA DSSTox DATA RELEASE OCTOBER 2015. At the time of toxEval package release, this information was found: https://www.epa.gov/chemical-research/exploring-toxcast-data-downloadabl in the section marked "Download ToxCast Chemical Information". This was in the "ToxCast & Tox21 Chemicals Distributed Structure-Searchable Toxicity Database (DSSTox files)" data set.

Value

data frame with columns: "Substance_Name","Substance_CASRN", "Structure_MolWt"

Examples

```
head(tox_chemicals)
```

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