

# Package: wqbench (via r-universe)

September 17, 2024

**Title** Calculate Aquatic Life Benchmarks

**Version** 0.2.0

**Description** Download recent versions of the US EPA ECOTOX database.  
Clean, standardize and classify data so values are comparable.  
Use a SSD or deterministic method to determine the critical toxicity value and assessment factors to compute the aquatic life water quality benchmark for a compound.

**License** Apache License (== 2)

**Imports** bcddata, chk, chktemplate, DBI, dplyr, ggplot2, httr, readr, rlang, RSQLite, rvest, scales, ssdtools (>= 1.0.6.9011), stringr, tibble, tidyr, utils, withr

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*combine\_bc\_species*      *Combine BC Species and DB Species*

**Description**

Internal to allow for testing

**Usage**

```
combine_bc_species(bc_species, db_species)
```

**Arguments**

```
bc_species      A data frame
db_species      A data frame
```

**Value**

A data frame

**Examples**

```
## Not run:
data <- combine_bc_species(bc_species, db_species)

## End(Not run)
```

*combine\_bc\_wqg*      *Combine BC Water Quality Guidelines with DB Chemicals*

**Description**

Internal to allow for testing

**Usage**

```
combine_bc_wqg(bc_wqg, db_chemicals)
```

**Arguments**

bc\_wqg            A data frame  
db\_chemicals    A data frame

**Value**

A data frame

**Examples**

```
## Not run:  
data <- combine_bc_wqg(bc_wqg, db_chemicals)  
  
## End(Not run)
```

---

combine\_concentration\_endpoints

*Combine the Concentration Endpoints list to db endpoints*

---

**Description**

Internal to allow for testing

**Usage**

```
combine_concentration_endpoints(endpoint_concentration_pick, db_endpoint_code)
```

**Arguments**

endpoint\_concentration\_pick  
                          A data frame  
db\_endpoint\_code  
                          A data frame

**Value**

A data frame

**Examples**

```
## Not run:  
data <- combine_concentration_endpoints(  
  endpoint_concentration_pick, db_endpoint_code  
)  
  
## End(Not run)
```

---

`combine_conc_conversions`*Combine Concentration Unit Conversation Values with DB Concentration Unit*

---

**Description**

Internal to allow for testing

**Usage**

```
combine_conc_conversions(concentration_std, db_concentration_unit_codes)
```

**Arguments**

```
concentration_std  
  A data frame  
db_concentration_unit_codes  
  A data frame
```

**Value**

A data frame

**Examples**

```
## Not run:  
data <- combine_conc_conversions(  
  concentration_std, db_concentration_unit_codes  
)  
  
## End(Not run)
```

---

`combine_duration_conversions`*Combine Duration Unit Conversation Values and DB duration unit*

---

**Description**

Internal to allow for testing

**Usage**

```
combine_duration_conversions(duration_std, db_duration_unit_codes)
```

**Arguments**

duration\_std    A data frame  
db\_duration\_unit\_codes  
                  A data frame

**Value**

A data frame

**Examples**

```
## Not run:  
duration_unit_codes_std <- combine_duration_conversions(  
  duration_std, db_duration_unit_codes  
)  
  
## End(Not run)
```

---

combine\_lifestage        *Combine Life Stage Groups and db life stage*

---

**Description**

Internal to allow for testing

**Usage**

```
combine_lifestage(lifestage_codes, db_lifestage_codes)
```

**Arguments**

lifestage\_codes  
                  A data frame  
db\_lifestage\_codes  
                  A data frame

**Value**

A data frame

**Examples**

```
## Not run:  
lifestage_groups <- combine_lifestage(lifestage_codes, db_lifestage_codes)  
  
## End(Not run)
```

---

combine_media	<i>Combine Media Type Coding</i>
---------------	----------------------------------

---

**Description**

Internal to allow for testing

**Usage**

```
combine_media(db_media_type)
```

**Arguments**

db\_media\_type A data frame

**Value**

A data frame

**Examples**

```
## Not run:  
media_type <- combine_media(db_media_type)  
  
## End(Not run)
```

---

combine_trophic_group	<i>Combine Trophic Groups and DB species</i>
-----------------------	--

---

**Description**

Internal to allow for testing

**Usage**

```
combine_trophic_group(trophic_groups, db_species)
```

**Arguments**

trophic\_groups A data frame  
db\_species A data frame

**Value**

A data frame

## Examples

```
## Not run:  
species_trophic_group <- combine_trophic_group(trophic_groups, db_species)  
  
## End(Not run)
```

---

join\_data

*Join Data*

---

## Description

Internal to wqb\_join\_data() to allow for testing.

## Usage

```
join_data(  
  db_results,  
  db_tests,  
  db_endpoint_codes,  
  db_species,  
  db_lifestage_codes,  
  db_chemicals,  
  db_duration_unit_codes,  
  db_concentration_unit_codes,  
  db_references,  
  db_effect_codes,  
  db_media_type_codes,  
  db_meta_data_download  
)
```

## Arguments

db_results	A data frame
db_tests	A data frame
db_endpoint_codes	A data frame
db_species	A data frame
db_lifestage_codes	A data frame
db_chemicals	A data frame
db_duration_unit_codes	A data frame
db_concentration_unit_codes	A data frame
db_references	A data frame



```
db_effect_codes
      A data frame
db_media_type_codes
      A data frame
db_meta_data_download
      A data frame
```

**Value**

Invisible data frame

**Examples**

```
## Not run:
data <- wqb_join_data(
  db_results, db_tests, db_endpoint_codes, db_species, db_lifestage_codes,
  db_chemicals, db_duration_unit_codes, db_concentration_unit_codes,
  db_references, db_effect_codes, db_media_type_codes, db_meta_data_download
)
## End(Not run)
```

---

read_bc_species	<i>Read in BC Species CSV</i>
-----------------	-------------------------------

---

**Description**

Internal to allow for testing

**Usage**

```
read_bc_species(bc_species_file_path, db_species)
```

**Arguments**

```
bc_species_file_path
      A file path
db_species           A data frame
```

**Value**

A data frame

**Examples**

```
## Not run:
data <- read_bc_species(bc_species_file_path, db_species)
## End(Not run)
```

---

read\_bc\_wqg                      *Read BC Water Quality Guidelines*

---

**Description**

Internal to allow for testing

**Usage**

```
read_bc_wqg(db_chemicals)
```

**Arguments**

db\_chemicals    A data frame

**Value**

A data frame

**Examples**

```
## Not run:  
chemicals_bc_wqg <- read_bc_wqg(db_chemicals)  
  
## End(Not run)
```

---

read\_concentration\_endpoints  
                                  *Read the Concentration Endpoints*

---

**Description**

Internal to allow for testing

**Usage**

```
read_concentration_endpoints(conc_endpoints_file_path, db_endpoint_code)
```

**Arguments**

conc\_endpoints\_file\_path  
                                  A file path  
db\_endpoint\_code  
                                  A data frame

**Value**

A data frame

**Examples**

```
## Not run:
endpoint_concentration <- read_concentration_endpoints(
  conc_endpoints_file_path, db_endpoint_code
)

## End(Not run)
```

---

read\_conc\_conversions *Read Concentration Unit Conversation Values*

---

**Description**

Internal to allow for testing

**Usage**

```
read_conc_conversions(concentration_std_file_path, db_concentration_unit_codes)
```

**Arguments**

```
concentration_std_file_path
  A file path
db_concentration_unit_codes
  A data frame
```

**Value**

A data frame

**Examples**

```
## Not run:
concentration_unit_codes_std <- read_conc_conversions(
  concentration_std_file_path, db_concentration_unit_codes
)

## End(Not run)
```

---

`read_duration_conversions`*Read Duration Unit Conversation*

---

**Description**

Internal to allow for testing

**Usage**

```
read_duration_conversions(duration_std_file_path, db_duration_unit_codes)
```

**Arguments**

```
duration_std_file_path  
    A file path  
db_duration_unit_codes  
    A data frame
```

**Value**

A data frame

**Examples**

```
## Not run:  
duration_unit_codes_std <- read_duration_conversions(  
  duration_std_file_path, db_duration_unit_codes  
)  
  
## End(Not run)
```

---

`read_lifestage`*Read Life Stage Groups*

---

**Description**

Internal to allow for testing

**Usage**

```
read_lifestage(lifestage_file_path, db_lifestage_codes)
```

**Arguments**

lifestage\_file\_path  
                                  A data frame  
db\_lifestage\_codes  
                                  A data frame

**Value**

A data frame

**Examples**

```
## Not run:  
lifestage_groups <- read_lifestage(lifestage_file_path, db_lifestage_codes)  
  
## End(Not run)
```

---

read\_trophic\_group     *Read Trophic Groups and DB species*

---

**Description**

Internal to allow for testing

**Usage**

```
read_trophic_group(trophic_groups_file_path, db_species)
```

**Arguments**

trophic\_groups\_file\_path  
                                  A file path  
db\_species                   A data frame

**Value**

A data frame

**Examples**

```
## Not run:  
species_trophic_group <- read_trophic_group(trophic_groups_file_path, db_species)  
  
## End(Not run)
```

---

 template

*Template for Adding your own Data*


---

**Description**

Template for Adding your own Data

**Usage**

template

**Format**

A data.frame with columns:

**name** Row description.

**latin\_name** The latin name of the test species.

**endpoint** Toxicity endpoint.

**effect** The effect that was being tested.

**lifestage** The lifestage the species was during the test.

**effect\_conc\_mg.L** Contaminant concentration that corresponds to the endpoint.

**effect\_conc\_std\_mg.L** The effect concentration standardized to include the acute to chronic ratio to extrapolate acute and/or effect concentrations to chronic and/or no-effect concentrations in mg/L.

**trophic\_group** Trophic group of species.

**ecological\_group** Identification of salmonids and planktonic invertebrates. If neither of these, listed as “other”.

**species\_present\_in\_bc** Species is present in British Columbia if entry = TRUE

---

 wqb\_add\_bc\_species

*Add BC Species*


---

**Description**

Read in a list of British Columbia species and add a column to the species table in the database to indicate if the species is present in British Columbia.

**Usage**

wqb\_add\_bc\_species(database, quiet = FALSE)

**Arguments**

database        A string to the location of the database.  
quiet            Turn off message when quiet set to TRUE.

**Details**

The BC species data is contained in a csv file in the extdata folder of the package. This file can be edited by adding new species or removing species. Do not add new columns, rename columns or rename the file. The file must only contain a single column named `latin_name`.

The `latin_name` column must consist of the genus and species separated by a space. The `latin_name` column in the `bc-species.csv` file is matched to the `latin_name` column in the `species` table of the database. A new column `species_present_in_bc` is added to the `species` table that codes each species as TRUE if it matches a value in the `bc-species.csv` or FALSE if there is no match.

**Value**

Invisible data frame

**Examples**

```
## Not run:  
bc_species <- wqb_add_bc_species(  
  database = "ecotox_ascii_09_15_2022.sqlite"  
)  
  
bc_species <- wqb_add_bc_species(  
  database = "ecotox_db/ecotox_ascii_09_15_2022.sqlite"  
)  
  
## End(Not run)
```

---

wqb\_add\_bc\_wqg        *Add BC Water Quality Guidelines*

---

**Description**

Read in the British Columbia water quality guidelines (wqg) and add a column to the chemicals tables in the database to indicate if the chemical is present in the British Columbia water quality guidelines.

**Usage**

```
wqb_add_bc_wqg(database, quiet = FALSE)
```

**Arguments**

database        A string to the location of the database.  
quiet            Turn off message when quiet set to TRUE.

## Details

The wqg data is stored in the BC Data Catalogue.

The CAS\_number column in the bc wqg data is matched to the cas\_number column in the chemicals table of the database. A new column present\_in\_bc\_wqg is added to the chemicals table that codes each chemical as TRUE if the chemical is present in wqg or FALSE if the chemical is not present in wqg.

## Value

Invisible data frame

## Examples

```
## Not run:
chem_bc_wqg <- wqb_add_bc_wqg(
  database = "ecotox_ascii_09_15_2022.sqlite"
)

chem_bc_wqg <- wqb_add_bc_wqg(
  database = "ecotox_db/ecotox_ascii_09_15_2022.sqlite"
)

## End(Not run)
```

---

wqb\_add\_concentration\_endpoints  
*Add the Concentration Endpoints*

---

## Description

Read in the concentration endpoints that have been selected to keep in the final data set. Add a column to the endpoint\_codes table in the database to mark the corresponding endpoints.

## Usage

```
wqb_add_concentration_endpoints(database, quiet = FALSE)
```

## Arguments

database	A string to the location of the database.
quiet	Turn off message when quiet set to TRUE.



## Details

The list of concentration endpoints is contained in a csv file in the extdata folder of the package. The csv file can be edited by adding or removing rows. To add new rows get the code and description values from the endpoint\_codes table in the database and paste them into the csv file.

Do not add new columns, rename columns or rename the file. The file must only contain the code and description column.

The code values in the endpoint-concentration file are matched to the code values in the endpoint\_code table in the database. A new column concentration\_flag is added to the endpoint\_code table that codes each endpoint as TRUE if the endpoint is present in endpoint-concentration.csv file.

## Value

Invisible data frame

## Examples

```
## Not run:
wqb_add_concentration_endpoints(
  database = "ecotox_ascii_09_15_2022.sqlite"
)

wqb_add_concentration_endpoints(
  database = "ecotox_db/ecotox_ascii_09_15_2022.sqlite"
)

## End(Not run)
```

---

wqb\_add\_conc\_conversions

*Add Concentration Unit Conversation Values*

---

## Description

Read in the concentration-conversion file and code units that can be converted and which ones will be removed. Three columns will be added to the concentration\_unit\_codes table in the database, indicate which units are being kept, the conversion factor, and the units it is being converted to. Currently units are converted to mg/L or equivalent.

## Usage

```
wqb_add_conc_conversions(database, quiet = FALSE)
```

## Arguments

database	A string to the location of the database.
quiet	Turn off message when quiet set to TRUE.

**Details**

The list of units to be converted are contained in a csv file in the extdata folder of the package. The csv file can be edited by adding or removing rows. To add new rows get the code and description values from the concentration\_unit\_codes table in the database and paste them into the csv file.

Do not add new columns, rename columns or rename the file. The file must only contain the columns: code, description, conc\_conversion\_flag, conc\_conversion\_value\_multiplier and conc\_conversion\_unit.

The conc\_conversion\_flag column indicates which units are being converted and which are being removed because they can not be converted or are not in the aquatic portion of the data. The conc\_conversion\_value\_multiplier column contains the value need to convert the unit into the unit listed in the conc\_conversion\_unit column.

The code values in the concentration-conversion file are matched to the code values in the concentration\_unit\_codes table in the database.

**Value**

Invisible data frame

**Examples**

```
## Not run:
concentration_unit_code_standardization <- wqb_add_conc_conversions(
  database = "ecotox_ascii_09_15_2022.sqlite"
)

concentration_unit_code_standardization <- wqb_add_conc_conversions(
  database = "ecotox_db/ecotox_ascii_09_15_2022.sqlite"
)

## End(Not run)
```

---

wqb\_add\_duration\_conversions

*Add Duration Unit Conversation Values*

---

**Description**

Read in the duration-conversion file and code unit values that can be converted and which ones will be removed. Two columns will be added to the duration\_unit\_codes table in the database to indicate which units are being kept and the conversion factor. Currently duration units are converted to hours.

**Usage**

```
wqb_add_duration_conversions(database, quiet = FALSE)
```

**Arguments**

database            A string to the location of the database.  
 quiet                Turn off message when quiet set to TRUE.

**Details**

The list of units to be converted are contained in a csv file in the extdata folder of the package. The csv file can be edited by adding or removing rows. To add new rows get the code and description values from the duration\_unit\_codes table in the database and paste them into the csv file.

Do not add new columns, rename columns or rename the file. The file must only contain the columns: code, description, duration\_units\_to\_keep and duration\_value\_multiplier\_to\_hours.

The code values in the duration-conversion file are matched to the code values in the duration\_unit\_codes table in the database.

The duration\_units\_to\_keep column indicates which units are being converted and which are being removed because they can not be converted or are not in the aquatic portion of the data. The duration\_value\_multiplier\_to\_hours column contains the value need to convert the unit into hours.

**Value**

Invisible data frame

**Examples**

```
## Not run:
duration_unit_code_standardization <- wqb_add_duration_conversions(
  database = "ecotox_ascii_09_15_2022.sqlite"
)

duration_unit_code_standardization <- wqb_add_duration_conversions(
  database = "ecotox_db/ecotox_ascii_09_15_2022.sqlite"
)

## End(Not run)
```

---

wqb\_add\_lifestage            *Add Life Stage Groups*

---

**Description**

Read in the life stage simple groups and add a column in the lifestage\_code table in the database to mark the corresponding values.

**Usage**

```
wqb_add_lifestage(database, quiet = FALSE)
```

**Arguments**

database        A string to the location of the database.  
 quiet           Turn off message when quiet set to TRUE.

**Details**

Only life stages related to fish or amphibians have been coded. The purpose of the coding is to be able to simplify the many life stages into three categories: els (early life stage), juveniles and adults. Not all life stages have been coded into these three groups.

The life stage data is contained in a csv file in the extdata folder of the package. The csv file can be edited by adding or removing rows. To add new rows get the code and description values from the `lifestage_code` table in the dataset and paste them into the csv file and then add the value to the `simple_lifestage` column.

Do not add new columns, rename columns or rename the file. The file must only contain the code, `description_lifestage` and `simple_lifestage` column.

The code values in the `lifestage-codes.csv` file are matched to the code values in the `lifestage_code` table in the database. Any codes that match are coded in a new column called `simple_lifestage`.

**Value**

Invisible data frame

**Examples**

```
## Not run:
lifestage_codes <- wqb_add_lifestage(
  database = "ecotox_ascii_09_15_2022.sqlite"
)

lifestage_codes <- wqb_add_lifestage(
  database = "ecotox_db/ecotox_ascii_09_15_2022.sqlite"
)

## End(Not run)
```

---

wqb\_add\_media

*Add Media Type Coding of Salt or Fresh Water*


---

**Description**

Code the media type information into three categories: salt water, fresh water and not reported.

**Usage**

```
wqb_add_media(database, quiet = FALSE)
```

**Arguments**

database        A string to the location of the database.  
quiet            Turn off message when quiet set to TRUE.

**Details**

Read in the media\_type\_codes table from the database and code the 24 groups into three categories: salt water, fresh water or not reported. The new categories are added to a column in the table called media\_type\_group.

**Value**

Invisible data frame

**Examples**

```
## Not run:  
media_info <- wqb_add_media(  
  database = "ecotox_ascii_09_15_2022.sqlite"  
)  
  
media_info <- wqb_add_media(  
  database = "ecotox_db/ecotox_ascii_09_15_2022.sqlite"  
)  
  
## End(Not run)
```

---

wqb\_add\_trophic\_group *Add Trophic Groups to Database*

---

**Description**

Read in the trophic and ecological groups and add a column to the species table in the database that lists the groups for each species.

**Usage**

```
wqb_add_trophic_group(database, quiet = FALSE)
```

**Arguments**

database        A string to the location of the database.  
quiet            Turn off message when quiet set to TRUE.

**Details**

The trophic group data is contained in a csv file in the extdata folder of the package. This file can be edited by adding or removing groups and classes. Do not add new columns, rename columns or rename the file.

The trophic groups file must contain the columns: class, order, trophic\_group, and ecological\_group. The class and order columns are matched to the class and tax\_order columns in the species table of the database and then adds the trophic\_group and ecological\_group columns to the species table.

**Value**

Invisible data frame

**Examples**

```
## Not run:
trophic_group <- wqb_add_trophic_group(
  database = "ecotox_ascii_09_15_2022.sqlite"
)

trophic_group <- wqb_add_trophic_group(
  database = "ecotox_db/ecotox_ascii_09_15_2022.sqlite"
)

## End(Not run)
```

---

wqb\_af

*Determine the Assessment Factors*

---

**Description**

Determines the species variation factor, ecological assessment factor and B.C. species factor.

**Usage**

```
wqb_af(data)
```

**Arguments**

data            A data frame

**Details**

This is a wrapper function that calls wqb\_af\_bc\_species(), wqb\_af\_ecological() and wqb\_af\_variation().

**Value**

A data frame

**Examples**

```
## Not run:  
data <- wqb_af(data)  
  
## End(Not run)
```

---

wqb_af_bc_species	<i>Determine the BC Species Assessment Factor</i>
-------------------	---

---

**Description**

Determines an assessment factor based on the number of BC species present.

**Usage**

```
wqb_af_bc_species(data)
```

**Arguments**

data	A data frame
------	--------------

**Details**

Check the resource document for how the assessment factor was calculated.

**Value**

A data frame

**Examples**

```
## Not run:  
data <- wqb_af_bc_species(data)  
  
## End(Not run)
```

---

wqb\_af\_ecological      *Determine the Ecological Assessment Factors*

---

**Description**

Determines the assessment factor based on the presence of certain ecological groups.

**Usage**

```
wqb_af_ecological(data)
```

**Arguments**

data                      A data frame

**Details**

Check the resource document for how the assessment factor was calculated.

**Value**

A data frame

**Examples**

```
## Not run:  
data <- wqb_af_ecological(data)  
  
## End(Not run)
```

---

wqb\_af\_variation      *Determine the Species Variation Assessment Factor*

---

**Description**

Determine the assessment factor based on the number of trophic groups and species.

**Usage**

```
wqb_af_variation(data)
```

**Arguments**

data                      A data frame



**Details**

Check the resource document for how the assessment factor was calculated.

**Value**

A data frame

**Examples**

```
## Not run:  
data <- wqb_af_variation(data)  
  
## End(Not run)
```

---

wqb\_aggregate

*Aggregate Data for each Species*

---

**Description**

Aggregate data to select the most sensitive value for each species. The priority of effect level depends on the benchmark method that will be used.

**Usage**

```
wqb_aggregate(data)
```

**Arguments**

data            A data frame

**Details**

Check the resource document for the rules used to aggregate the data down to a single value per species. This is Step 5.

**Value**

A data frame

**Examples**

```
## Not run:  
data <- wqb_aggregate(data)  
  
## End(Not run)
```

---

wqb\_benchmark\_method *Determine Benchmark Method*

---

### Description

Determine if a species sensitivity distribution (SSD) or deterministic method will be used to determine the aquatic life water quality benchmark value for the data. A column called method will be added to the data indicating which method will be used.

### Usage

```
wqb_benchmark_method(data)
```

### Arguments

data            A data frame

### Details

Check the resource document for the rules used to determine which benchmark method will be used. This is Step 4.

### Value

A data frame

### Examples

```
## Not run:  
data <- wqb_benchmark_method(data)  
data <- wqb_benchmark_method(agggregated_data)  
  
## End(Not run)
```

---

wqb\_check\_add\_data *Check the Uploaded Data*

---

### Description

Checks the uploaded data for the basic requirements to ensure the data matches the downloaded Ecotox data.

### Usage

```
wqb_check_add_data(data, template)
```

**Arguments**

`data` A data frame. The data you want to check.  
`template` A data frame. The format the data should be in, in the `chktemplate` format.

**Details**

The values for the `endpoint`, `trophic_group`, and `ecological_group` columns are checked against the data tables used to build the database. To update the allowed values the corresponding csv file needs to be updated.

**Value**

A data frame

**Examples**

```
## Not run:  
data <- wqb_check_add_data(data, template)  
  
## End(Not run)
```

---

wqb\_classify\_duration *Classify Duration*

---

**Description**

Classify each test as either acute or chronic in the `duration_class` column.

**Usage**

```
wqb_classify_duration(data, quiet = FALSE)
```

**Arguments**

`data` A data frame  
`quiet` Turn off message when quiet set to TRUE.

**Details**

Check the resource document for the rules used to determine the classification for each trophic group. This is Step 2.

**Value**

A data frame

**Examples**

```
## Not run:  
classified_data <- wqb_classify_duration(compiled_data)  
  
## End(Not run)
```

---

wqb_clean_data	<i>Compile Data</i>
----------------	---------------------

---

**Description**

Join database tables together and start filtering and cleaning data.

**Usage**

```
wqb_clean_data(data, quiet = FALSE)
```

**Arguments**

data	A data frame.
quiet	Turn off message when quiet set to TRUE.

**Details**

Check the resource document more details on the data added, filter conditions and cleaning steps.  
This is part of Step 1.

**Value**

Invisible data frame

**Examples**

```
## Not run:  
data <- wqb_clean_data(data)  
  
## End(Not run)
```

---

wqb\_create\_data\_set     *Create the Data Set for the App*

---

## Description

This function downloads the data, creates and adds all the data to the database, compiles, standardizes, and classifies the data. The output of this function is fed into the app.

## Usage

```
wqb_create_data_set(  
  file_path = "~/Ecotoxicology/ecotox",  
  version = 1,  
  folder_path = "~/Ecotoxicology/ecotox_db/",  
  quiet = FALSE,  
  ask = TRUE,  
  save_rds = TRUE  
)
```

## Arguments

file_path	A string of the file path location to save the downloaded files. The default is your current working directory.
version	An integer to indicate which version you want to download. The default is 1 which downloads the most recent version.
folder_path	Folder path to write to.
quiet	Turn off message when quiet set to TRUE.
ask	Turn off question when set to FALSE.
save_rds	Saves the data set as a rds file in the folder_path. Turn off when set to FALSE.

## Value

A data frame

## Examples

```
## Not run:  
wqb_create_data_set(  
  file_path = "~/Ecotoxicology/ecotox",  
  version = 1,  
  folder_path = "~/Ecotoxicology/ecotox_db/"  
)  
  
## End(Not run)
```

---

wqb\_create\_epa\_ecotox *Create the ECOTOX Database*

---

**Description**

Create a SQLite database from the US EPA ECOTOX downloaded files.

**Usage**

```
wqb_create_epa_ecotox(folder_path = ".", data_path, quiet = FALSE, ask = TRUE)
```

**Arguments**

folder_path	Folder path to write to.
data_path	Folder path to the downloaded ECOTOX folder
quiet	Turn off message when quiet set to TRUE.
ask	Turn off question when set to FALSE.

**Details**

This functions reads in the text files in the folder and writes them to the database.

This function will overwrite a database if already present.

**Value**

Invisible string of the file path of the database.

**Examples**

```
## Not run:  
wqb_create_epa_ecotox(data_path = "ecotox_ascii_12_15_2022")  
  
## End(Not run)
```

---

wqb\_download\_epa\_ecotox

*Download ECOTOX Data Files*

---

**Description**

Download the ECOTOX data files from their FTP website. The default is to download the most recent version of the data.

## Usage

```
wqb_download_epa_ecotox(  
  file_path = ".",  
  version = 1,  
  ask = TRUE,  
  quiet = FALSE  
)
```

## Arguments

file_path	A string of the file path location to save the downloaded files. The default is your current working directory.
version	An integer to indicate which version you want to download. The default is 1 which downloads the most recent version.
ask	Turn off question when set to FALSE.
quiet	Turn off message when quiet set to TRUE.

## Details

You have the option of downloading older version of the data but only up to the four most recent version. The most recent version is set as 1 and the oldest version is version 4.

The downloaded folder will contain various files that are needed to build the database.

You must have a working internet connection to run this function successfully.

## Value

Invisible string of the file path the downloaded files were saved.

## References

US EPA ECOTOX website: <https://cfpub.epa.gov/ecotox/>

Olker, J. H., Elonen, C. M., Pilli, A., Anderson, A., Kinziger, B., Erickson, S., Skopinski, M., Pomplun, A., LaLone, C. A., Russom, C. L., & Hoff, D. (2022). The ECOTOXicology Knowledgebase: A Curated Database of Ecologically Relevant Toxicity Tests to Support Environmental Research and Risk Assessment. *Environmental Toxicology and Chemistry*, 41(6):1520-1539. <https://doi.org/10.1002/etc.5324>

## Examples

```
## Not run:  
wqb_download_epa_ecotox()  
  
wqb_download_epa_ecotox("data_download")  
  
# pull previous version of the database  
wqb_download_epa_ecotox("data_download", version = 2)  
  
## End(Not run)
```

---

wqb\_filter\_chemical     *Filter to a Single Chemical*

---

**Description**

Filter to a Single Chemical

**Usage**

```
wqb_filter_chemical(data, cas_num)
```

**Arguments**

data	A data frame
cas_num	A string of the cas number.

**Value**

A data frame

**Examples**

```
## Not run:  
data <- wqb_filter_chemical(data, "129909906")  
data <- wqb_filter_chemical(data, "1000984359")  
  
## End(Not run)
```

---

wqb\_generate\_ctv     *Generate Critical Toxicity Value*

---

**Description**

Determine the critical toxicity value for the species. The function will apply the method listed in the method column.

**Usage**

```
wqb_generate_ctv(data, dists = ssdtools::ssd_dists_bcanz())
```

**Arguments**

data	A data frame
dists	A character vector of the distributions to fit.



**Details**

The `ctv_est_mg.L` is the estimate of the critical toxicity value for the species. The `ctv_lcl_mg.L` is the lower confidence limit. The `ctv_ucl_mg.L` is the upper confidence limit.

The Deterministic method will always produce missing values in the `ctv_lcl_mg.L` and `ctv_ucl_mg.L` columns.

**Value**

A data frame

**Examples**

```
## Not run:  
ctv <- wqb_generate_ctv(data)  
  
## End(Not run)
```

---

wqb_join_data	<i>Join Data</i>
---------------	------------------

---

**Description**

Join database tables together and start filtering and cleaning data.

**Usage**

```
wqb_join_data(database, quiet = FALSE)
```

**Arguments**

database	A string to the location of the database.
quiet	Turn off message when quiet set to TRUE.

**Details**

Check the resource document more details on the data added, filter conditions and cleaning steps. This is part of Step 1.

**Value**

Invisible data frame

**Examples**

```
## Not run:
data_compiled <- wqb_join_data(
  database = "ecotox_ascii_09_15_2022.sqlite"
)

data_compiled <- wqb_join_data(
  database = "ecotox_db/ecotox_ascii_09_15_2022.sqlite"
)

## End(Not run)
```

---

wqb_method_det	<i>Deterministic Method to Generate Critical Toxicity Value for the Chemical</i>
----------------	--

---

**Description**

Use the deterministic method to generate the critical toxicity value for the data set.

**Usage**

```
wqb_method_det(data)
```

**Arguments**

data	A data frame
------	--------------

**Details**

Check the resource document for more details . This is Step 1.

**Value**

A data frame

**Examples**

```
## Not run:
bench_iodine <- wqb_method_det(data)

## End(Not run)
```

---

`wqb_method_ssd`*SSD Method to Calculate Critical Toxicity Value for the Chemical*

---

**Description**

Use a species sensitivity distribution to calculate the critical toxicity value for the data set. The critical toxicity value is the hazardous concentration for 5% of species (HC5) when the SSD method is used.

**Usage**

```
wqb_method_ssd(data, fit, nboot = 1000)
```

**Arguments**

<code>data</code>	A data frame
<code>fit</code>	The fit
<code>nboot</code>	The number of bootstrap samples. Default value of 1000.

**Details**

A wrapper on the `ssdtools` package function `ssdtools::ssd_hc_bcanz()` that only returns the HC5 concentration.

**Value**

A data frame

**Examples**

```
## Not run:  
hc5 <- wqb_method_ssd(data, fit)  
  
## End(Not run)
```

---

`wqb_plot`*Plot Data*

---

**Description**

Plot the standardized data to see the concentrations per species for each endpoint.

**Usage**

```
wqb_plot(data)
```

**Arguments**

data            A data frame

**Examples**

```
## Not run:  
wqb_plot(data)  
  
## End(Not run)
```

---

wqb\_plot\_det            *Plot the Deterministic Method Results*

---

**Description**

Plot deterministic results to see the standardized data, critical toxicity value and aquatic life benchmark.

**Usage**

```
wqb_plot_det(data)
```

**Arguments**

data            A data frame

**Examples**

```
## Not run:  
wqb_plot_det(data)  
  
## End(Not run)
```

---

wqb\_plot\_ssd            *Plot Species Sensitivity Distribution*

---

**Description**

Plot results to see the species sensitivity distribution. The dashed line shows the HC5 value.

**Usage**

```
wqb_plot_ssd(data, fit)
```

**Arguments**

data	A data frame
fit	The fit from <code>ssd</code>

**Details**

This is a wrapper on `ssdtools::predict()` and `ssdtools::ssd_plot()`.

**Examples**

```
## Not run:  
wqb_plot_ssd(data, fit)  
  
## End(Not run)
```

---

wqb_ssd_fit	<i>Fit BCANZ Distributions</i>
-------------	--------------------------------

---

**Description**

Wrapper to `ssdtools::ssd_fit_bcanz()`. The `sp_aggre_conc_mg.L` values are the concentrations used.

**Usage**

```
wqb_ssd_fit(data, dists = ssdtools::ssd_dists_bcanz())
```

**Arguments**

data	A data frame
dists	A character vector of the distributions to fit

**Value**

A data frame

**Examples**

```
## Not run:  
fit <- wqb_ssd_fit(data)  
  
## End(Not run)
```

---

`wqb_ssd_hc5`*Run SSD to get Hazard Concentrations*

---

**Description**

Wrapper to the `ssdtools::ssd_hc_bcanz()` function and selects only the row which is 5%.

**Usage**

```
wqb_ssd_hc5(fit, nboot = 1000)
```

**Arguments**

<code>fit</code>	The fit from <code>ssd</code>
<code>nboot</code>	A count of the number of bootstrap samples to use to estimate the SE and confidence limits. Default value of 1000.

**Details**

The number of bootstrap samples is set to 1000 so the estimates are quick to generate. Check out [ssdtools::ssd\\_hc\\_bcanz\(\)](#) for more details.

**Value**

A data frame

**Examples**

```
## Not run:  
hc5 <- wqb_ssd_hc5(fit)  
  
## End(Not run)
```

---

`wqb_standardize_effect`*Standardize type of Effect*

---

**Description**

Determine and apply factor needed to standardize the endpoints.

**Usage**

```
wqb_standardize_effect(data, quiet = FALSE)
```

**Arguments**

data            A data frame  
 quiet           Turn off message when quiet set to TRUE.

**Details**

Check the resource document for details the rules used to determine standardized the endpoints. This is Step 3.

**Value**

A data frame

**Examples**

```
## Not run:
standardized_effect_data <- wqb_standardize_effect(data)
standardized_effect_data <- wqb_standardize_effect(classified_data)

## End(Not run)
```

---

wqb\_summary\_af

*Summary Table of the Assessment Factor Values*


---

**Description**

Create summary table of the species variation factor, ecological assessment factor and B.C. species factor.

**Usage**

```
wqb_summary_af(data)
```

**Arguments**

data            A data frame

**Value**

A data frame

**Examples**

```
## Not run:
summary_af <- wqb_summary_af(data)

## End(Not run)
```

---

wqb\_summary\_trophic\_groups

*Summary Table of Assessment Factors Information*

---

**Description**

Summary Table of Assessment Factors Information

**Usage**

```
wqb_summary_trophic_groups(data)
```

**Arguments**

data            A data frame

**Value**

A data frame

**Examples**

```
## Not run:  
summary_af <- wqb_summary_trophic_groups(data)  
  
## End(Not run)
```

---

wqb\_summary\_trophic\_species

*Summary Table of Number of Species per Trophic Group*

---

**Description**

Summary Table of Number of Species per Trophic Group

**Usage**

```
wqb_summary_trophic_species(data)
```

**Arguments**

data            A data frame

**Value**

A data frame.



**Examples**

```
## Not run:  
summary_trophic <- wqb_summary_trophic_species(data)  
  
## End(Not run)
```

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