

US EPA TOXCAST DATA RELEASE SEPTEMBER 2023 Database & tcpl R Package

This file describes the contents of the September 2023 ToxCast data release. The database/R package download consists of the following files:

`invitrodb_v4_1_mysql.gz`

Invitrodb Database Loading

To utilize the database, the user must have access to a MySQL server and load the database contained in the “`invitrodb_v4_1_mysql.gz`” file. The file is a zipped sql file containing the entire invitrodb database. To avoid errors while calling large queries, we recommend the MySQL server setting, ‘`max_allowed_packet`’, is set to at least 1 GB.

More comprehensive documentation for installing MySQL and creating a database from sql dump files can be found online: <https://dev.mysql.com/doc/>.

tcpl Package Installation

The R software package `tcpl` is available on CRAN <https://cran.r-project.org/web/packages/tcpl/index.html> and GitHub <https://github.com/USEPA/CompTox-ToxCast-tcpl>. Given `tcplLite` is no longer supported by `tcpl`, a MySQL connection is required for use. For standalone curve-fitting without connectivity to the MySQL database `invitrodb`, see the R software package dependency `tcplfit2`, on CRAN <https://cran.r-project.org/web/packages/tcplfit2/index.html> and GitHub <https://github.com/USEPA/CompTox-ToxCast-tcplFit2>.

To install `tcpl`, the user will first need to properly install Rtools, enabling R to compile the source package. The package relies on R ($\geq 3.5.0$), and the following packages: `data.table` ($\geq 1.9.4$), `DBI`, `RMariaDB`, `numDeriv`, `RColorBrewer`, `utils`, `stats`, `methods`, `graphics`, `grDevices`, `sqldf`, `dplyr`, `tidyr`, `plotly`, `tcplfit2`, `ggplot2`, `gridExtra`, `stringr`. To interact with the MySQL database, the user may want to use the `RMySQL` package in addition to queries via `tcpl` functions.

The package can be installed from CRAN using the following R command:

```
install.packages("tcpl")
```

For the most current development version of `tcpl`, run the following R command:

```
devtools::install_github("USEPA/CompTox-ToxCast-tcpl")
```

Vignettes can be found on CRAN at <https://cran.r-project.org/web/packages/tcpl/index.html>, for a comprehensive overview of ToxCast processing and data retrieval. The introductory vignette also includes an appendix with definitions of all database fields.

For questions or concerns, please contact Jason Brown (brown.jason@epa.gov) or Madison Feshuk (madison@epa.gov).