

shinyssd v1.0: Species Sensitivity Distributions for Ecotoxicological Risk Assessment

María Florencia D'Andrea^{1,2} and Julie Céline Brodeur^{1,2}

1 Consejo de Investigaciones Científicas y Técnicas (CONICET), Ciudad Autónoma de Buenos Aires, Buenos Aires, Argentina. 2 Instituto de Recursos Biológicos. Centro de Investigaciones de Recursos Naturales (CIRN). Instituto Nacional de Tecnología Agropecuaria (INTA), Hurlingham, Buenos Aires, Argentina.

DOI: 10.21105/joss.00785

Software

■ Review 🗗

■ Repository 🗗

■ Archive 🗗

Submitted: 31 May 2018 Published: 29 May 2019

License

Authors of papers retain copyright and release the work under a Creative Commons Attribution 4.0 International License (CC-BY).

Summary

Living organisms have different sensitivities to toxicants. This variability can be represented by constructing a species sensitivity distribution (SSD) curve, whereby the toxicity of a substance to a group of species is described by a statistical distribution. Building the SSD curve allows calculating the Hazard Concentration 5% (HC_5), that is, the concentration at which 5% of the considered species are affected. The HC_5 is widely used as an environmental quality criterion and a tool for ecological risk assessment (Posthuma, Suter II, & Traas, 2001).

The shinyssd web application is a versatile and easy to use tool that serves to simultaneously model the SSD curve of a user-defined toxicity dataset based on four different statistical distribution models (log-normal, log-logistic, Weibull, Pareto). shinyssd directly calculates three estimators HC_1 , HC_5 and HC_{10} associated to the four distribution models together with its confidence intervals, allowing the user to select the statistical distribution and associated HC values that best adjust the dataset.

The level of confidence of the results obtained from a SSD curve will depend on the number of species used to produce the SSD. In this sense, the first tab of the user interface is used for visualizing the number of species for which toxicological data are available for each toxicant, species group, and endpoint combination in the uploaded dataset. A minimum of species is necessary to build a SSD curve varies according to the literature (Belanger et al., 2016; Newman et al., 2000; Plant Protection Products & Residues, 2013; Wheeler, Grist, Leung, Morritt, & Crane, 2002).

After selecting the toxicant and species groups, the user can filter and select subsets of data from the whole database by applying different quality criteria (e.g., if the studies reported a chemical confirmation of the concentrations of the toxicant tested). The values entered in each column of the database serve as categories to filter the database in relation to characteristics of the bioassays. The final SSD curve is fitted to different distributions using the package fitdistribus and actuar. The HC is estimated for all the distributions.

By facilitating and streamlining toxicity data analysis and the creation of SSD curves, the user interface proposed here should be useful for environmental managers and regulators conducting ecological risk assessments and scientific research.

Information for Users

• shinyssd includes a preloaded database with a quatic toxicological data for the pesticides Cypermethrin and Glyphosate. This data was extracted of the ECOTOX



database of the Environmental Protection Agency of the United States (EPA). An external comma-separated values file (.csv) could be uploaded by the user according to the format of the template.csv file attached in the repo.

- There is a warning alert message if you are entering data with different units, to avoid conflictive results.
- shinyssd includes the option of download the relevant results as a .docx report.
- shinyssd is optimized for browser use.
- The app can be run from R using the following code:

library(devtools)

devtools::install_github("flor14/shinyssd", subdir = "shinyssd")

library(shinyssd)

shinyssd::shinyssd_run()

Community guidelines

Report Issues:

• Questions, feedback, bug reports: please open an issue in the issue tracker of the project.

Contribution to the software:

• Please open an issue in the issue tracker of the project that describes the changes you would like to make to the software and open a pull request with the changes. The description of the pull request must references the corresponding issue.

Acknowledgements

We wish to thank Ana Diedrichs, the R community and R-Ladies for their help and support.

References

Belanger, S., Brill, J., Rawlings, J., McDonough, K., Zoller, A., & Wehmeyer, K. (2016). Aquatic toxicity structure-activity relationships for the zwitterionic surfactant alkyl dimethyl amine oxide to several aquatic species and a resulting species sensitivity distribution. *Ecotoxicology and environmental safety*, 134, 95–105. doi:10.1016/j.ecoenv.2016.08.023

Newman, M., Ownby, D., Mézin, L., Powell, D., Christensen, T., Lerberg, S., & Anderson, B. (2000). Applying species-sensitivity distributions in ecological risk assessment: Assumptions of distribution type and sufficient numbers of species. *Environmental Toxicology and Chemistry: An International Journal*, 19(2), 508–515. doi:10.1002/etc. 5620190233



Plant Protection Products, E. P. on, & Residues. (2013). Guidance on tiered risk assessment for plant protection products for aquatic organisms in edge-of-field surface waters. $EFSA\ Journal,\ 11(7),\ 3290.\ doi:10.2903/j.efsa.2013.3290$

Posthuma, L., Suter II, G., & Traas, T. (2001). Species sensitivity distributions in ecotoxicology. CRC press. doi:10.1201/9781420032314

Wheeler, J., Grist, E., Leung, K., Morritt, D., & Crane, M. (2002). Species sensitivity distributions: data and model choice. *Marine Pollution Bulletin*, 45(1-12), 192-202. doi:10.1002/etc.5620190233