

Abstract:

The major challenge in ecological risk assessment is to assess the hazard exposure in various trophic species residing in different environmental compartments. The species sensitivity distributions (SSDs) reflect the difference in observations of chemical sensitivity among different modeled species. The reliance on animals for ecological risk assessment (ERA) of nanoparticles (NPs) is a heated topic of debate among various regulatory agencies. Thus, animal dependence should be minimized to the lowest possible threshold using intelligent testing strategies (ITS), including various *in silico* tools. *In silico* tools, such as quantitative-structure-activity relationship (QSAR) and read-across (RA) approaches, link molecular descriptors that interpret chemical structural properties with their biological activity. Computational tools have long been used in NPs toxicity prediction and data gap filling. However, no effort has been made to develop SSD estimation models employing acute and chronic toxicity data against multiple species. Additionally, the available models hold a restricted application and can only be applied to assess the ecotoxicity of a single kind/group of species owing to their limited chemical, biological and taxonomic domain. The current project will address the limitations of all these existing models. Still, it will also propose several new models against various sub-groups of NPs following strict OECD guidelines for model development. A “class-specific” read-across technique will be used to fill missing data points. In the second approach, the collected toxicity data against various sub-groups of NPs will be used to check and identify the best performing read-across technique available for different chemical classes termed as “class-specific”. The “class-specific” analysis results will be used to propose a novel and better performing read-across technique validated on a large studied dataset. Finally, the resource outcomes of the project will be incorporated into a knowledge database and software tool, which will be made available on the dedicated website.