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Chemometric modeling of toxicity of contaminants of emerging concern to *Dugesia japonica* and its interspecies correlation with daphnia and fish: QSTR and i-QSTTR approaches

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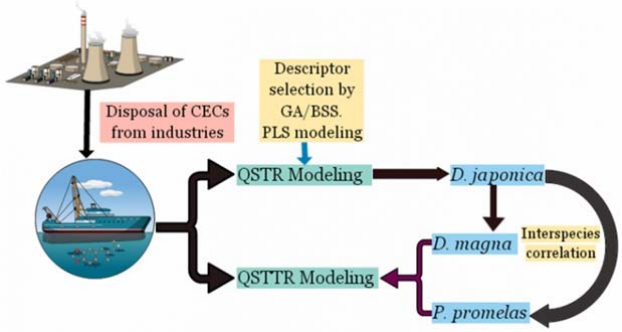
Graphical Abstract



Abstract

With increasing population of the world, the uses of needful chemicals are also increasing day by day. In the last 20 years, thousands of research papers have been published, reporting different aspects of chemicals known as contaminants of emerging concern (CEC), and more than 40,000 chemicals are identified as CECs. The pharmaceuticals and personal care products (PPCPs), endocrine disrupting chemicals (EDCs), UV filters etc. belong to the CEC class and their incorrect disposal procedure has made them as emerging contaminants. CECs are detected in the groundwater which may produce undesirable effects to human health and aquatic organisms. Unfortunately, very less amount of data are available on the environmental behavior and ecotoxicity of pharmaceuticals and other CECs; therefore, we need computational models for ecotoxicological risk assessment of chemicals with speed and accuracy that may fill the data gap by utilizing fewer resources and experimental animals. New approaches like Quantitative Structure-Activity Relationship (QSAR) may be able to generate

	valuable information and could help to meet these challenges. In this present study, we have developed Quantitative Structure-Toxicity Relationship (QSTR) models for the prediction of aquatic ecotoxicity of CECs on fresh water planarian (*Dugesia japonica*) by partial least squares (PLS) regression algorithm using simple molecular descriptors selected by genetic algorithm approach. Furthermore, interspecies quantitative structure toxicity-toxicity relationship (QSTTR) models were developed between planarian and daphnia (*Daphnia magna*) as well as between planarian and fish (*Pimephales promelas*) which can extrapolate data from one toxicity endpoint to another toxicity endpoint. The descriptors were calculated from PaDEL-Descriptor and Dragon software. Both QSTR and QSTTR models have desirable statistical qualities, meeting rigorous criteria of different validation metrics and OECD guidelines. Applicability domain assessment was also carried out to define the scope of the developed models and to highlight the compounds which are falling outside the domain. Consensus predictions were also performed based on multiple models generated in this study by using the Intelligent Consensus Predictor (ICP) tool http://teqip.jdvu.ac.in/QSAR_Tools/DTCLab/) to enhance the prediction quality for external set compounds. This study shows how in silico models can be applied for the toxicity assessment of CECs in aquatic organisms and indicating what are the structural features involved in their toxicity.

References

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