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Application of computational methods to predict aquatic toxicity of pesticides

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PURPOSE OF THE ABSTRACT

Pesticides have found numerous applications in the agricultural and health industries. They allow for increased crop production and ultimately economic growth, while also controlling disease-carrying pests, which can have adverse effects on public health. However, pesticides can also be major contaminants of groundwater and waterways, demonstrating the importance of robust screening methods to limit any unintended environmental and human harm prior to commercialization and use. This research evaluates two in silico methods for predicting eco-toxicity, which were previously developed by us, on a group of prominent pesticides and their metabolites. The first model uses a rule of three which applies octanol-water distribution coefficient, band gap and molecular volume parameters to define a safe space, a chemical space that encompasses chemicals benign to aquatic species. Additionally, the CADRE-AT (Computer- Aided Discovery and Redesign for aquatic toxicity) system, which was recently extended to afford continuous (vs. categorical) predictions of toxicity, was used to predict acute mean lethal concentration values for each pesticide, and the results were compared with experimental values. These two models were developed for commercial chemicals; however, they were not assessed for performance on pesticides, specifically. When applying the rule of three, our results placed all pesticides with experimental data in their appropriate category, i.e. safe vs. toxic to aquatic species. The CADRE-AT approach inaccurately predicted three chemicals, placing each in a neighboring category of the correct category of concern. These chemicals were further examined for their toxicity mechanisms and metabolic transformations to develop new strategies to improve the performance of the model. Overall, our results show that the two in silico approaches examined are sufficiently robust and of relevance to both industry and regulatory decision makers in assessing environmental hazard associated with pesticides. These computational methods provide a fast and economically efficient method for screening pesticides before distribution so that their efficacy can be optimized, while minimizing unintended harm to environmental health.

FIGURES

FIGURE 1

FIGURE 2

KEYWORDS
toxicity prediction | safer chemicals | pesticide toxicity

BIBLIOGRAPHY