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Use of QSAR Validation Principles to Enhance Predictive Approaches in the US EPA ECOSAR Model

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Abstract:
The US EPA Office of Pollution Prevention and Toxics (OPPT) is responsible for implementing the Toxic Substances Control Act (TSCA). TSCA is the US law that regulates industrial chemicals in the US and OPPT evaluates both new chemicals entering commerce, as well as those chemicals that have been in existence for some time. In evaluating new and existing chemicals over the past 35+ years, OPPT has developed a strong knowledge base in structure-activity relationships (SARs). The Ecological Structure Activity Relationships (ECOSAR) Class Program is a computerized predictive system that estimates aquatic toxicity. The program estimates a chemical's acute (short-term) toxicity and chronic (long-term or delayed) toxicity to aquatic organisms based on their structural similarity to chemicals for which aquatic studies are available. Model development is continuous and dependent on availability of new data and information submitted to the US EPA or generated within the scientific community.

Recent work was completed in ECOSAR version 1.1 to better represent toxicity data of pesticidal compounds within the model and enhance the chemical space of the tool. Following the OECD QSAR validation principles, the US EPA's Office of Research and Development conducted an independent validation of the ECOSAR version 1.1 QSAR models using a set of chemicals having an acute mode of action of acetylcholinesterase inhibition. The resulting case study titled 'Use of ECOSAR QSAR Models to Estimate the Acute Toxicity of Organophosphate and Carbamate Pesticide Classes to Fish Species' found that the carbamates esters performed reasonably well, but highlighted the need for improvement of chemical categories and models for the phosphate esters. EPA reviewed additional data, chemical diversity, and use classes (e.g., pesticidal activities versus phosphate esters used in industrial applications like flame retardants) within the training sets to identify ways to improve the QSAR relationships. The US EPA will present these results along with updated QSAR regression analysis for the phosphate esters.

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