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Modeling the Toxicity of Phenols to Algae: A 'QSAR' Perspective

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Evaluation of data from toxicity tests using microalgae is an integral part of environmental risk assessment. Accordingly, the new chemical management system of Europe, namely the REACH legislation (Registration, Evaluation, Authorization and Restriction of Chemicals), requires ecotoxicity data on algae for compounds manufactured or imported into the European Community > 1 ton/annum. Taking into account the huge number of compounds that needs to be evaluated for risk assessment, REACH also encourages the use of alternative methods to laboratory testing, such as the Quantitative Structure – Activity Relationships (QSARs), to predict the toxicity of untested chemicals.

Despite their ecological significance and in contrast to the regulatory needs, ecotoxicity data on algae are scarce. Therefore, there is an urgent requirement to develop fast and reliable methods to reduce the data gap in algal ecotoxicity. In an attempt to demonstrate how QSAR methodology can be incorporated into ecotoxicity studies with the aim of predicting the adverse effects of untested chemicals, a case study on the toxicity of phenols to algae will be presented.





