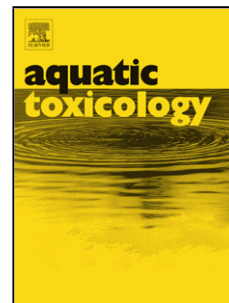


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Title: A Bayesian network model for predicting aquatic toxicity mode of action using two dimensional theoretical molecular descriptors

Author: John F. Carriger Todd M. Martin Mace G. Barron



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Highlights

- * A Bayesian network was developed to classify chemical mode of action (MoA)
- * The network was based on the aquatic toxicity MoA for over 1000 chemicals
- * A Markov blanket algorithm selected a subset of theoretical molecular descriptors
- * Sensitivity analyses found influential descriptors for classifying the MoAs
- * Overall precision of the Bayesian MoA classification model was 80%

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