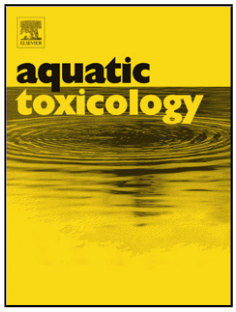

Title: A Bayesian network model for predicting aquatic toxicity mode of action using two dimensional theoretical molecular descriptors

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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%