

In silico estimation of aquatic species sensitivity using QSAR and Web-ICE

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Determining the sensitivity of a diversity of species to environmental contaminants continues to be a significant challenge in ecological risk assessment because toxicity data are generally limited to a few standard species. In many cases, QSAR models are used to estimate toxicity in the absence of multiple species toxicity values. We developed species sensitivity distributions (SSDs) and fifth percentile hazard levels (HC5) for aquatic species using three USEPA QSAR tools: ECOSAR (Ecological Structure Activity Relationships; www.epa.gov/oppt/newchems/tools/21ecosar.htm), ASTER (Assessment Tools for the Evaluation of Risk; www.epa.gov/med/Prods_Pubs/aster.htm), and T.E.S.T. (Toxicity Estimation Software Tool; <http://www.epa.gov/nrmrl/std/cppb/qsar/>). QSAR estimates were used as input into the SSD module of the internet-based toxicity estimation program Web-ICE (<http://www.epa.gov/ceampubl/fchain/webice/>). In silico estimated HC5s were compared to HC5s developed from a dataset of over 14,000 toxicity records extracted from Ecotox and other sources. Preliminary results indicated that the input LC50 values generated by the three QSAR tools were often substantially higher estimates of toxicity, resulting in less protective Web-ICE generated HC5s than HC5s generated from measured toxicity data. Using two surrogate species for taxa-specific toxicity estimates did not significantly improve HC5 when compared with measured toxicity SSDs. In general, chemicals with narcosis-based MOAs had the best agreement between measured and in silico estimated HC5s. Additional research will determine those chemical classes and MOA with the most accurate QSAR estimates of species sensitivity.