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Title: An Online QSAR Prediction Platform to Support the Environmental Sciences

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Historical QSAR models are currently utilized across a broad range of applications within the U.S. Environmental Protection Agency (EPA). These models predict basic physicochemical properties (e.g., logP, aqueous solubility, vapor pressure), which are then incorporated into exposure, fate and transport models. Whereas the classical manner of publishing results in peer-reviewed journals remains appropriate, there are substantial benefits to be gained by providing enhanced, open access to the training data sets and resulting models. Benefits include improved transparency, more flexibility to expand training sets and improve model algorithms, and greater ability to independently characterize model performance both globally and in local areas of chemistry. We have developed a web-based prediction platform that uses open-source descriptors and modeling algorithms, employs modern cheminformatics technologies, and is tailored for ease of use by the toxicology and environmental regulatory community. This tool also provides web-services to meet both EPA's projects and the modeling community at-large. The platform hosts models developed within EPA's National Center for Computational Toxicology, as well as those developed by other EPA scientists and the outside scientific community. Recognizing that there are other on-line QSAR model platforms currently available which have additional capabilities, we connect to such services, where possible, to produce an integrated hub for accessing existing models and their predictions. Whereas our specific efforts are focused on applications to environmental sciences, the platform is developed in a manner that will allow for the general hosting of models for physicochemical prediction, toxicity prediction and, ultimately, could house hybrid QSAR models for chemical-biology data streams to serve our general mission at EPA's National Center for Computational Toxicology. This abstract does not reflect U.S. EPA policy.