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Poster presentation

QSAR modelling of acute toxicity in the fathead minnow

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There are more than 70000 chemicals in use today and many more being synthesized. It is vital to assess the influence of these compounds on the environment and on human health. Experimental testing is both time-consuming and expensive, and accordingly, there is a pressing requirement for accurate *in silico* methods to assess the toxicity. QSAR studies of the environmental fate of chemicals are widely used for this purpose. One of the broadly used toxicity database is the Distributed Structure-Searchable Toxicity (DSSTox) database from the U.S. Environmental Protection Agency (http://www.epa.gov). It provides various data including EPA Fathead Minnow Aquatic Toxicity Database (EPAFHM), which currently contains structures of 617 chemicals of which 580 structures have toxicity data (EPAFHM_v3b_617_10Apr2006). The toxicity end-points are based on the 96 h LC50 (mmol/L) values for the fathead minnow, which used for standard toxicity test described by the U.S. Environmental Protection Agency. We used QNA (Quantitative Neighbourhoods of Atoms) descriptors and Self-Consistent Regression for QSAR modeling of acute toxicity in the fathead minnow. The statistical parameters of the correlation are the follows: N = 580, R^2 = 0.804, F = 32.508, SD = 0.670, Q^2 = 0.759. For 522 compounds (90%), the deviation of the predicted values from the observed ones is less than 1 logLC50 (mmol/L). Leave-10%-out cross-validation procedure was used for assessment of prediction ability of the method. It was performed 20 times and average R^2 of prediction was 0.606, the highest value of R^2 = 0.815, the lowest value of R^2 = 0.501. Applicability domain was estimated for test set by leave-10%-out cross-validation procedure. These results confirmed robustness and satisfactory predictive ability of the method, hence, it can be used for computational assessment of acute toxicity in new compounds.