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QSTR modeling based on multiple linear regression for acute toxicity prediction of phenol derivatives against Tetrahymena pyriformis

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Abstract: In this work, the modeling of inhibitory grown activity against Tetrahymena pyriformis is described. The 0-2D Dragon descriptors based on structural aspects to gain some knowledge of factors influencing aquatic toxicity are mainly used. Besides, it is done by an enlarged data of phenol derivatives describe for the first time. It overcomes the previous datasets with about one hundred compounds. Moreover, the results of the model evaluation by the parameters in the training, prediction and validation provide adequate results comparable with those of the previous works. The more influential descriptors involved in the model are: X3A, MWC02, MWC10 and piPC03 with positive contributions to the dependent variable; and MWC09, piPC02 and TPC with negative influences. In a next step, a median-size database of nearly 8,000 phenolic compounds extracted from ChEMBl was evaluated with the quantitative-structure toxicity relationship (QSTR) model developed providing some clues (SARs) for identification of ecotoxicological compounds. The outcome of this report are very useful to screen chemical databases in use for finding the compounds responsible of aquatic contamination in the biomarker used in the current work.