World Academy of Science, Engineering and Technology
International Journal of Physical and Mathematical Sciences
Vol:10, No:02, 2016

Estimation of the Acute Toxicity of Halogenated Phenols Using Quantum Chemistry Descriptors

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Abstract : Phenols and especially halogenated phenols represent a substantial part of the chemicals produced worldwide and are known as aquatic pollutants. Quantitative structure–toxicity relationship (QSTR) models are useful for understanding how chemical structure relates to the toxicity of chemicals. In the present study, the acute toxicities of 45 halogenated phenols to Tetrahymena Pyriformis are estimated using no cost semi-empirical quantum chemistry methods. QSTR models were established using the multiple linear regression technique and the predictive ability of the models was evaluated by the internal cross-validation, the Y-randomization and the external validation. Their structural chemical domain has been defined by the leverage approach. The results show that the best model is obtained with the AM1 method (R^2= 0.91, R^2CV= 0.90, SD= 0.20 for the training set and R^2= 0.96, SD= 0.11 for the test set). Moreover, all the Tropsha' criteria for a predictive QSTR model are verified.

Keywords : halogenated phenols, toxicity mechanism, hydrophobicity, electrophilicity index, quantitative stucture-toxicity relationships
Conference Title : ICMCC 2016 : International Conference on Mathematical and Computational Chemistry
Conference Location : Istanbul, Türkiye
Conference Dates : February 15-16, 2016