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Department of Chemistry

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(In the field of Analytical Chemistry)

Prediction of phenolic properties of some phenol derivatives by using pure quantum descriptors and applying QSAR Methods

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Abstract

In this work attempt were done to construct a local quantitative structure activity relationships between the phenolic properties of 67 phenol derivatives and their corresponding quantum mechanical variables of charge, dipole, electrostatic potential and orbital energy. As follows, all molecular structures were produced and optimized in HyperChem and Guassian98 softwares on theoretical level of HF/6-31g basis function. Where the Isolated and in solvent (water and octanol) interactions, using onzagre reaction field model, were considered. Besides, carbon-13 chemical shifts for those carbon atoms only situated on the parent molecule were calculated using HF/6-31g NMR=giao keyword in Guassian98. Multivariate linear regression with correlation coefficient of R^2_{LOO}=0.43 reveals that LUMO variable show significant effect on phenolic activity (Log(1/C) of all phenol derivatives. As our preliminary studies proposes two different trend of mechanisms for data set, the modeling was extended for two 51 and 16 groups separately. Where, their corresponding linear correlation coefficient models obtained to be R^2_{LOO}=0.64 and =0.7, respectively. Although the two different models were obtained, the LUMO variable in both models shows a significant contribution. In another attempt, to bring all phenol derivatives in the same regime, an artificial neural network in conjunction with Genetic algorithm variable selection model was employed. An excellent correlation coefficient (R^2=0.79) with respect to the previous one was achieved. In present model, highest positive charge, besides orbital energy governs the activity. Therefore, models propose that the phenolic activity performs through charge exchange between the phenol derivatives and target molecules. It is believed that the substituent stabilize the phenol ring through inductive and/or resonance mechanism are more favorable in increasing phenolic properties.

Keywords: Phenolic activity; QSAR; Phenol derivatives; quantum parameters.