مدیریت تحصیلات تکمیلی

دانشکده علوم

گروه شیمی

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Abstract

In this project, a local quantitative–structure activity relationship study was conducted to evaluate and predict the Hydrophobicity (Clog P) and biological activity (IC_{50}) of 19 molecules of 6-amino-4-phenyltetrahydroquinoline derivatives. In this manner, the molecular structures were produced and optimized in HyperChem and Guassian98 softwares, respectively. Where the Isolated and in solvent (water and octanol) interactions, using onzagre reaction field model, were considered. Four different classes of quantum mechanical features including charge, dipole, electrostatic potential and orbital energy were calculated. Furthermore, carbon-13 chemical shifts for those carbon atoms only situated on the parent molecule were calculated using HF/3-21g NMR=giao keyword in Guassian98. Multivariate linear regression model was used to explore the relevant variables affecting the Hydrophobicity (Clog P) and biological activity (IC_{50}) in term of quantum variables. Their corresponding linear correlation coefficient models obtained to be $R2_{LOO}$=0.8724 and 0.6136 , respectively. Based on resulted model, hydrophobicity of the 6-amino-4-phenyltetrahydroquinoline derivatives are prefer less polar media with low hydrogen bonding strength, the weaker the hydrogen bonds the higher the hydrophobicity. Also, the model achieved for biological activity (IC_{50}) proposes that the substitutes which increase the chemical shift of the carbon number 4 on the parent molecule would be of highly interest in future synthesis of more effective 6-amino-4-phenyltetrahydroquinoline derivatives.

Keywords: quantitative–structure activity relationship, 6-amino-4-phenyltetrahydroquinoline derivatives, hydrophobicity, biological activity, multivariate linear regression,