QSPR models to Predict the quantum chemical properties of imidazole derivatives using genetic algorithm multiple linear regression and back-propagation-artificial neural network

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April 21, 2022

Abstract

Imidazole derivatives are the foundation of different types of drugs with a wide range of biological activities. In this study, the genetic algorithm multiple linear regression (GA- MLR), and backpropagation-artificial artificial neural network (BP-ANN) were applied to design QSPR models to predict the quantum chemical properties like the entropy(S) and enthalpy of formation([?]Hf) of imidazole derivatives. In order to draw molecular structure of 84 derivative compounds Gauss View 05 program was used. These structures were optimized at DFT-B3LYP / 6-311G* level with Gaussian09W. The Dragon software was used to calculate a set of different molecular descriptors, and the genetic algorithm procedure and backward stepwise regression were applied for the selection of descriptors. The resulting quantitative GA-MLR model of [?]Hf, showed that there is good linear correlation between the selected descriptors and [?]Hf of compounds. Also the results show that the BP-ANN model appeared to be superior to GA-MLR model for prediction of entropy. Different internal and external validation metrics were adopted to verify the predictive performance of QSPR models. The predictive powers of the models were found to be acceptable. Thus, these QSPR models may be useful for designing new series of imidazole derivatives and prediction of their properties.

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