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Prediction of Acidity Constants of Thiazolidine-4-carboxylic Acid Derivatives Using Ab Initio and Genetic Algorithm-partial Least Squares

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Abstract: A quantitative structure-property relationship study is suggested for the prediction of the acidity constants of some thiazolidine-4-carboxylic acid derivatives in aqueous solution. Ab initio theory was used to calculate some quantum chemical descriptors, including electrostatic potentials and local charges at each atom, highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) energies, etc. Modeling of the acidity constant of thiazolidine-4-carboxylic acid derivatives as a function of molecular structures was established by means of the partial least squares algorithm. The subset of descriptors, which resulted in a low prediction error, was selected by genetic algorithm. This model was applied for the prediction of the acidity constant of some thiazolidine-4-carboxylic acid derivatives, which were not in the modeling procedure. Relative errors of prediction lower than 1.5% were obtained by using the genetic algorithm-partial least squares (GA-PLS) method. The developed model has good prediction ability with a root mean square error of prediction of 0.0419 and 0.1013 for PLS and GA-PLS models, respectively.

Key Words: Ab initio, partial least squares, genetic algorithm, acidity constant, thiazolidine-4-carboxylic acid

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