QSPR Study of the Complex Formation Constants between β-cyclodextrin and Some Organic Compounds

Cyclodextrins (CDs) are a group of structurally related natural products and also known as cycloamylosis. Recently CDs have been utilized in many different fields such as catalysis, separation science and technology, drug delivery, pharmaceutical application, food, personal careproducts and etc\[1\]. The purpose of this study is to construct a quantitative structure-property relationship (QSPR) model that is able to predict the stability between different guest molecules and β-cyclodextrin. This study is performed using the bee algorithm (BA) and the adaptiveneuro-fuzzy inference system (ANFIS). The 3-D structures of 34 compounds \[1\] were optimized using HyperChem software (version 8.0) with semi empirical AM\[1\] optimization method. After optimization a total of 2244, 162, 24, and 3-D descriptors were generated using Dragon software (version 3.0) \[2\]. In the first, bee algorithm program was written in Matlab in our laboratory by the authors and then was used to select the most important descriptors. Descriptor selection procedure starts with flying of n scout bees toward N-dimensional search space of N descriptors \[3\]. Then the formation constants and error values are calculated using selected descriptors and multiple linear regression model. Finally, the best descriptors are selected due to the less calculated errors. Therefore on the basis of BA, five descriptors were selected and applied as input to the network of the ANFIS. Finally, to evaluate the predictive power of bee-ANFIS the optimized model was applied to all dataset (training, test and validation sets). RMSEs of 0.7956, 0.4143 and 0.4444 were obtained for the training, test and validation sets, respectively. The correlation of coefficient were obtained as 0.9427, 0.871, and 0.9676 for training, test and validation sets, respectively.

Keywords: β-Cyclodextrin, QSPR, Bee Algorithm, ANFIS
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