عنوان مقاله:

A comparative QSAR study of aryl-substituted isobenzofuran-1(3H)-ones inhibitors

محل انتشار:

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نویسندگان:

Zahra Rostami - *Department of Chemistry, Payame Noor University (PNU), P. O. Box, ۱۹۳۹۵-۳۶۹۷ Tehran), Iran*

Eslam Pourbasheer - *Department of Chemistry, Payame Noor University (PNU), P.O. Box ۱۹۳۹۵-۳۶۹۷, Tehran, Iran*

خلاصه مقاله:

A comparative workflow, including linear and non-linear QSAR models, was carried out to evaluate the predictive accuracy of models and predict the inhibition activity of a series of aryl-substituted isobenzofuran-1(3H)-ones. The data set consisted of 34 compounds was classified into the training and test sets, randomly. Molecular descriptors were selected using the genetic algorithm (GA) as a feature selection tool. Various linear models based on multiple linear regression (MLR), principle component regression (PCR) and partial least square (PLS) and non-linear models based on artificial neural network (ANN), adaptive network-based fuzzy inference system (ANFIS) and support vector machine (SVM) methods were developed and compared. The accuracy of the models was studied by leave-one-out cross-validation (Q_LOO^2), Y-randomization test and group of compounds as external test set. Six descriptors were selected by GA to develop predictive models. With respect to the linear models, GA-PCR method was more accurate than the reset with statistical results of R_train^2=0.883, R_test^2=0.897, R_(adj,train)^2=0.829, R _(adj,test)^2=0.849, F_train=24.07 and F_test=34.17. In case of non-linear models, GA-SVM (R_train^2=0.992 and R_test^2=0.997) showed high predictive accuracy for the inhibitory activity. It was found that the selected descriptors .have the major roles in interpretation of biological activities of the compounds

کلمات کلیدی:

QSAR, genetic algorithms, global optimization, SVM