عنوان مقاله:

Study of Quantitative Structure-Activity Relationship (QSAR) of Diarylaniline Analogues as in Vitro Anti-HIV-۱ Agents in Pharmaceutical Interest

محل انتشار:

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خلاصه مقاله:

A study of quantitative structure-activity relationship (QSAR) is applied to a set of ۲۴ molecules derived from diarylaniline to predict the anti-HIV-۱ biological activity of the test compounds and find a correlation between the different physic-chemical parameters (descriptors) of these compounds and its biological activity, using principal components analysis (PCA), multiple linear regression (MLR), multiple non-linear regression (MNLR) and the artificial neural network (ANN). We accordingly proposed a quantitative model (non-linear and linear QSAR models), and we interpreted the activity of the compounds relying on the multivariate statistical analysis. The topological descriptors were computed with ACD/ChemSketch and ChemBioOffice۱۴.۰ programs. A correlation was found between the experimental activity and those obtained by MLR and MNLR such as (Rtrain = ۰.۸۸۶ ; R۲train = ۰.۷۸۶) and (Rtrain = ۰.۹۲۵ ; R۲train = ۰.۸۵۷) for the training set compounds, and (RMLR-test = ۰.۶) and (RMNLR-test = ۰.۷) for a randomly chosen test set of compounds, this result could be improved with ANN such as (R = ۰.۹۱۶ and R۲ = ۰.۸۴) with an architecture ANN (۶-۱-۱). To evaluate the performance of the neural network and the validity of our choice of descriptors selected by MLR and trained by MNLR and ANN, we used cross-validation method (CV) including (R = ۰.۹۰۳ and R۲ = ۰.۸۱۵) with the procedure leave-one-out (LOO). The results showed that the MLR and MNLR have served to predict activities, but when compared with the results given by a ۶-۱-۱ ANN model. We realized that the predictions fulfilled by the latter model were more effective than the other models. The statistical results indicated that this model is statistically significant and showing a very good stability towards the data variation in leave-one-out (LOO) cross validation.

کلمات کلیدی:

HIV-۱ virus, reverse transcriptase (RT), diarylaniline derivatives, QSAR, PCA