Using QSAR calculation in salicylanilide N-Alkil carbamates as anti Alzheimer drugs

Marya Golzar*,Dr. Ghasem Ghasemi,

In this work quantitative structure activity relationship (QSAR) study has been done on salicylanilide derivatives for the treatment of Alzheimer. Genetic algorithm (GA), artificial neural network (ANN), multiple linear regressions (stepwise-MLR) were used to create the nonlinear and linear QSAR models . For this purpose, ab initio geometry optimization performed at B3LYP level with a known basis set (6–31G). Hyperchem, chemoffice and gaussian 09W softwares were used for geometry optimization of the molecules and calculation of the quantum chemical descriptors. Finally, unscrambler program was used for analysis of data. The results obtained this work indicate that ANN model is the most favorable method toward the other statistical methods and exhibit reasonable prediction capabilities. General studies with GA-PCR methods, GA-PLS and jack-knife in different layers and different goals, compounds 1,16,17,18 and 20 among 20 studied compounds, have the lowest deviation and suggested as the best compounds to make anti-Alzheimer drugs. also the best descriptors are G1e، F02[C-N]، T(O..Cl)، GATS6m، GATS6p and Mor02m.

Keywords : Alzheimer, quantitative structure activity relationship (QSAR) , salicylanilide Compounds, Genetic Algorithm (GA), Artificial Neural Network (ANN).