I. Hdoufane [1]
I. Bjij [1]
D. Cherqaoui [1]

ARTIFICIAL NEURAL NETWORKS, SUPPORT VECTOR MACHINES AND DECISION TREES FOR ANTI HIV ACTIVITY PREDICTION OF ORGANIC COMPOUNDS

[1] Department of Chemistry, Faculty of Science Semlalia, BP 2390, Marrakech, Morocco

cherqaoui@uca.ma

Tetrahydroimidazo[4,5,1-jk][1,4]benzodiazepine (TIBO), as non-nucleoside analogues, constitute potent inhibitors of HIV-1 reverse transcriptase. In the present study, classification structure-activity relationship (SAR) models are developed to distinguish between high and low anti HIV inhibitors of these compounds. Different classifiers, such as support vector machines, artificial neural networks, random forests and decision trees have been established by using ten molecular descriptors. All models were validated with leave-one-out procedure and on an external test set. Randomization test was also conducted to ensure the robustness of the developed SAR models. The correct classification rate ranges from 93% to 100% and from 70% to 90% for the training and test sets, respectively. A comparison between all methods was done in order to evaluate their performances. The contribution of each descriptor was evaluated in order to understand the forces governing the activity of this class of compounds.

Keywords: structure activity relationship; TIBO; HIV inhibitors; support vector machines; decision trees; random forests and artificial neural networks.