

ABSTRACT

Human Immunodeficiency Virus (HIV) is a virus that can attack immune cells so that it can make a person more vulnerable to infections and other diseases. HIV is also an agent that causes Acquired ImmuneDeficiency Syndrome (AIDS). HIV-1 protease is one of the active targets found in research for the treatment of HIV. The use of existing HIV-1 protease inhibitors in AntiRetroviral Therapy (ART) also has an impact on mutations in the HIV virus that can cause resistance if used in long-term treatment. Thus, new HIV-1 protease inhibitors are needed to overcome this resistance problem. In this study, we aimed to develop a QSAR model to predict HIV-1 inhibitory activity using the gravitational search algorithm method. The gravitational search algorithm method is used to select molecular descriptors. We improve the performance of the model by performing hyperparameter adjustment procedures. From the results of the validation analysis, we found that model 3 contained 7 descriptors as the best model. This can be seen from the acquisition of the value obtained most in accordance with the validation parameter criteria where the r^2 value for training and test data are 0,84 and 0,82, respectively. The Q2 value for the leave-one-out cross-validation (LOO-CV) in the training data is 0,81.

Keywords : HIV-1 Protease Inhibitor, Quantitative Structure Activity Relationship (QSAR), Gravitational Search Algorithm (GSA), Neural Network (NN).