ABSTRACT

The spread of the SARS-CoV-2 virus in the COVID-19 disease outbreak took place very quickly. Currently, more than 200 million cases of COVID-19 have been confirmed. The ongoing outbreak caused a global economic recession that covered about hundreds of countries around the world. The current solution is the use of vaccines, but the mobility of the vaccines that have been created has not been maximized so that the role of drugs is very important in the process of mobilizing the vaccine. Of course acceleration is needed in the search for drugs to deal with COVID-19. The QSAR method is the right choice to accelerate the search for these drugs. This study focuses on making a QSAR prediction model making machine that predicts the in-house molecule of the Papain-like Protease (PLPro) inhibitor by using the ensemble method to form a model from several classifiers. The source of the training and test data is initially in the form of SMILES notation and then processed with the Mordred Descriptor program to convert it into a feature set from the data. Furthermore, data splitting is carried out from the dataset which will be used to make prediction models using the ensemble method. Then the model validation is carried out to get the results of the calculation of the numbers obtained from the confusion matrix. The results showed that the ensemble method was successfully implemented for the QSAR modeling system in the search for drugs for COVID-19 through PLPro inhibitors and the SARS-CoV-2 virus as the target.

Keywords: QSAR Study, Ensemble Method, PLPro inhibitor, SARS-CoV-2