Abstract

Malaria is a dangerous disease that often occurs in tropical regions and infects millions of people every year. Malaria infection in humans can be caused by the Plasmodium Falciparum parasite which enters the body from the bite of the Anopheles mosquito. This disease is very dangerous and is categorized as serious due to the continued discovery of parasite resistance to currently available anti-malarial drugs. Therefore, research on new anti-malarial drugs is urgently needed. This research was conducted to find new compounds that can inhibit the growth of the falcipain enzyme in the body, considering that this enzyme plays a very important role in the life cycle of the Plasmodium falciparum parasite. This research was conducted to find new compounds that can inhibit the growth of the falcipain enzyme in the body, considering that this enzyme plays a very important role in the life cycle of the Plasmodium falciparum parasite. The research was conducted using a computational-based approach using Quantitative Structured-Activity Relationship (QSAR) as research acceleration. The QSAR model will be built using the Particle Swarm Optimization algorithm as a feature selection method, and Regularized Linear Regression as a predictive model. The model validation results show that the best performance is produced by the Elastic Net model with an R^2 value in the training data of 0.813 and an R^2 value in the test data of 0.615. Then the value of the leave-one-out cross-validation (Q^2) obtained is 0.870.

Keywords: anti-malaria, falcipain, *particle swarm optimization* (PSO), *regularized linear regression* (RGR) *quantitative structure-activity relationship* (QSAR)