Prediksi Inhibitor Angiotensin-Converting-Enzyme (ACE) sebagai Agen Antihipertensi dengan Menggunakan Artificial Neural Network yang Dioptimalkan oleh Artificial Bee Colony

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Abstract

This study used a dataset from the ChEMBL database to predict the activity of Angiotensin-Converting Enzyme (ACE) inhibitors as antihypertensive agents using the Artificial Bee Colony (ABC) algorithm and Artificial Neural Network (ANN). Although time-consuming, expensive, and prone to uncertainty, traditional methods such as wet-lab testing are often employed for ACE inhibitor identification. This study aims to improve predictive performance by integrating systematic optimization through the ABC algorithm into ANN. The architectural and hyperparameters of the ANN model were optimized using the ABC algorithm. With an R^2 value of 0.683 on the test data, the model with a population size of 10 demonstrated the best performance among the five models evaluated, thus proving its efficacy in reflecting general data patterns. These results indicate the potential of integrating the ABC algorithm with ANN for more precise predictions of ACE inhibitor activity, offering a faster and more cost-effective alternative to conventional approaches. Larger and more diverse datasets are required for more in-depth research to confirm the generalizability of this method for various drug discovery purposes.

Keywords: artificial neural network, artificial bee colony, ace inhibitor, hypertension