

Implementasi Grey Wolf Algorithm pada Optimasi Metode Artificial Neural Network untuk Prediksi Toksisitas berbasis Fitur Fingerprint

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Abstract

Medicine is a primary need that is used to heal various diseases in living things. When consuming the drug alone, it may cause symptoms of toxicity. Therefore, it is very necessary to predict toxicity in chemical compounds that can be tolerated by the body. Regarding toxicity prediction, an alternative method is needed to replace High-Throughput Screening (HTS), because the method requires a lot of time and money. One of the alternative methods is using the machine learning method, such as Artificial Neural Network (ANN). This study aims to predict the toxicity of chemical compounds with feature-based fingerprints using the ANN method optimized by the grey wolf algorithm. According to the result, we obtained the best model from ANN with 2 hidden layers, tanh activation function, and adam optimizer, getting F1-score results and accuracy on test data with values of 0.590 and 0.887 respectively.

Keywords: *Deep learning, toxicity prediction, artificial neural network, grey wolf algorithm, fingerprint*
