

Abstract

Humans have the potential to be exposed to various types of chemical compounds, some of which are very dangerous for the body. Determination of the toxicity of a chemical is very important to minimize exposure to hazardous substances in everyday products. The method currently used to measure toxicity levels in large quantities is High-Throughput Screening (HTS). This experiment examines whether a chemical compound shows a certain level of toxicity. The disadvantages of using this method are that it takes too long and requires a large amount of money for research. Therefore, many experts suggest using other methods that can reduce these deficiencies. An alternative method that can be used is to implement the machine learning method to reduce the shortcomings of the previous HTS method. This study aims to predict toxicity using fingerprint datasets using the Artificial Neural Network method which is optimized using the cuckoo search algorithm. In this study, the best model results were obtained from the hidden layer 3 parameter with hidden node conditions [61, 69, 105], and the Relu activation function with an F1-Score and accuracy of 0.6153 and 0.9652, respectively.

Keywords: Toxicity, Fingerprint, Prediction, Artificial Neural Network, Cuckoo Search Algorithm