Abstract

Cancer, characterized by malignant cell development and uncontrolled division, resulted in 408,661 new cases and 242,988 deaths in Indonesia by 2022. Breast cancer was the most prevalent, accounting for 66,271 new cases or 16.2% of the total, followed by lung cancer with 38,904 cases (9.5%). Common cancer treatments include chemotherapy, surgery, radiotherapy, and drugs, with chemotherapy being the most prevalent despite its lack of selectivity and toxicity to healthy cells. However Polo-like kinase 1 (PLK1) has emerged as a promising anticancer target due to its critical role in cell cycle regulation. Currently, predicting PLK1 bioactivity relies on clinical trials, which are often time-consuming, costly, and inefficient. An alternative to predict bioactivity PLK1 using in silico methods because it is faster and more efficient. This study aims to develop a predictive model for PLK1 bioactivity using a Multilayer Perceptron (MLP) architecture, with Simulated Annealing (SA) algorithm employed for optimizing the architecture. The results showed that the MLP architecture optimized using the SA algorithm gave significant results. The best model obtained from MLP consists of 5 hidden layers with relu activation function and SGD optimizer, resulting the R^2 value and CC value at 0.68 and 0.84, respectively.

Keywords: cancer, plk1, predicting bioactivity, multilayer perceptron, simulated annealing