

Abstract

Cancer is one of the deadliest diseases in the world, with 1,665,540 people affected and 585,720 deaths annually. Cancer mortality is often caused by drug resistance. One method of treating cancer is traditional chemotherapy, but this method can damage healthy cells in the body. PLK1 is an anti-cancer agent that can be combined with existing chemotherapy. This anti-cancer agent has inhibitors that can be used for drug development. However, there are not many methods capable of identifying PLK1 inhibitors in cancer drug development. In this study, we aimed to predict the bioactivity of PLK1 inhibitors as anti-cancer agents using the Gravitational Search Algorithm (GSA) and Support Vector Machines (SVM). To optimize the model results, we used the GSA algorithm to select features with high correlation values. Furthermore, to improve the predictive accuracy of our model, hyperparameter tuning was applied to RBF, Polynomial, and Linear kernels. Through this rigorous process, we aimed to enhance the model's ability to accurately identify effective PLK1 inhibitors. Based on the results, it was found that the SVM model with the RBF kernel was more optimal in terms of prediction, with an R^2 value of 0.66 and a CC value of 0.83.

Keywords: *Cancer, PLK 1, Anti Cancer Agent, Gravitational Search Algorithm, Support Vector Machine*
