
In silico-based MMP-9 Inhibitors Prediction as Anti Cancer Therapeutics by using Particle Swarm Optimization-XGBoost Algorithm

Citra Aulia Sakinah¹, Isman Kurniawan²

^{1,2}Fakultas Informatika, Universitas Telkom, Bandung

¹citraauliasakinah@students.telkomuniversity.ac.id, ²ismankrn@telkomuniversity.ac.id

Abstract

Cancer remains a major global health concern, and matrix metalloproteinase-9 (MMP-9) is a key target in anti- cancer therapy due to its critical role in tumor progression and metastasis. In recent years, machine learning approaches have demonstrated significant potential in expediting the in silico drug discovery process. Nevertheless, further efforts are required to enhance the predictive accuracy of MMP-9 inhibitor bioactivity as part of cancer treatment strategies. This study aims to construct a predictive model for MMP-9 inhibitor bioactivity using machine learning by integrating Particle Swarm Optimization (PSO) for feature selection and XGBoost for classification. The dataset comprises 1,123 compounds labeled based on their IC₅₀ values and processed using PaDEL-Descriptor to extract molecular features. Three different PSO-based population schemes were evaluated to identify the most relevant subset of features that contribute to classification accuracy. Experimental results show that Scheme pop35 achieved the highest predictive performance, with a test accuracy and recall of 0.8210, precision of 0.8246, and F1- score of 0.8208. These findings indicate that combining PSO and XGBoost can effectively enhance the accuracy and robustness of in silico models, offering a promising strategy for the early identification of potential MMP-9 inhibitors in anti-cancer drug discovery.

Keywords: cancer, inhibitors mmp-9, particle swarm optimization, xgboost
