Prediction of MMP-9 Inhibitors as Anticancer Therapeutics by Using 1D-CNN Optimized by Monarch Butterfly Algorithm

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Abstract

The development of therapeutic drugs targeting MMP-9 inhibitors has shown potential in anticancer treatment. Matrix Metalloproteinase-9 (MMP-9) inhibitors are biomolecules that offer potential as novel anticancer therapies. The conventional development of therapeutic drugs for cancer faces significant challenges due to the high average cost, and an alternative solution is the use of Machine Learning. This study proposes a deep learning approach using a one-dimensional Convolutional Neural Network (1D-CNN) optimized with the Monarch Butterfly Optimization (MBO) algorithm to predict the activity of MMP-9 inhibitor compounds. The dataset consisted of 1,123 samples classified based on pIC50 values. Three baseline 1D-CNN architectures were evaluated and subsequently optimized through MBO with varying population sizes. The results demonstrate that deeper CNN architectures improve classification performance, while MBO significantly enhances convergence and accuracy. Among the optimization schemes, the third scheme, using a population size of 25, achieved the highest test accuracy of 0.7747 and F1-score of 0.7744, indicating superior generalization. These findings highlight the effectiveness of combining 1D-CNN and MBO for efficient and accurate anticancer compound prediction.

Keywords: Cancer, MMP-9 Inhibitor, MBO, 1-D CNN, Classification