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Re-evaluation and Validation of Graph Neural Network for Predicting Drug-Target Binding Affinity

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Abstract

In recent years, the increasing complexity of drug discovery has stimulated the need for advanced computational methods that can effectively predict drug-target interactions. Many and various methods are trying to be presented to improve the problem and reduce time and cost, and among these methods, the GraphDTA method using graph neural networks has succeeded in reducing the cost and time to provide new information.

In this paper, according to the dataset provided in GraphDTA, we measure the validity of this method using different evaluation criteria and prove its effectiveness. The results of applying different evaluation criteria to measure the accuracy of this method and to choose the best model in this case have been compared with each other.

Keywords: Bioinformatics, Predicting drug-target binding affinity, Graph Neural Networks

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