Implementasi Metode Algoritma Genetika-Random Forest pada Studi pada Inhibitor Diacylglycerol Acyltransferase-1(DGAT1) sebagai Anti Diabetes

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Abstract

Diabetes Mellitus (DM) is one of the most common chronic diseases suffered by the population in the world. DM is the fourth leading cause of death in developing countries. Treatment of diabetes is done by using drugs and blood sugar lowering therapy. However, the use of inappropriate drugs has side effects in long-term use, such as hypoglycemia and gastrointestinal disorders. One solution that is being tried is to use an inhibitor of the Diacylglycerol Acyltransferase-1 (DGAT-1) enzymes. In the theory of computational drug discovery, Quantitative Structure-Activity Relationship (QSAR) has been successfully created to accelerate the drug discovery process of biopharmaceutical properties of compounds that have not been tested. Build a QSAR model for predicting the activity of DGAT1 inhibitors as an anti-diabetic target by using the ensemble method. The ensemble method used in this study is Random Forest, AdaBoost, and Gradient Boosting. The best results are obtained by using a gradient boosting model with accuracy and the f1-score are 0,80 and 0,82 respectively.

Keywords: AdaBoost, Diabetes Mellitus, Genetic Algorithm, Gradient Boosting, Quantitative Structure-Activity Relationship (QSAR), Random Forest