QSAR Study on Diacylgycerol Acyltransferase-1 (DGAT-1) Inhibitor as Anti-diabetic using PSO-SVM Methods

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Abstract

Diabetes mellitus is a chronic disease that can occurred to anyone. Up until now, there are no specific drugs that have been found which can completely cure diabetes. One of the possible steps to treat diabetes mellitus is by inhibiting the growth of Diacylglycerol Acyltransferase-1 (DGAT-1) enzyme. This study aims to build a QSAR model on DGAT-1 inhibitors as anti-diabetic using Particle Swarm Optimization (PSO) and Support Vector Machine (SVM). Acyl-CoA: DGAT1 is a mikrosomal enzyme in lipogenesis which is increased in metabolically active cells to meet nutrient requirements. Microsomal enzymes that have an important in the triglyceride synthesis process of 1,2-diacylglycerol by catalyzing-acyl coa dependent acylations as anti-diabetics. The dataset used in this study consists of 228 samples containing molecular structures and their inhibitor activities. We reduce the number of features by removing features with a standard deviation less than the threshold value, followed by the PSO algorithm. The best-predicted result is obtained through the implementation of SVM with RBF kernel, with the score of $R^{\&}_{tra\$n}$ *and* $R^{\&}_{test}$ *are 0.75 and 0.67, respectively.*

Keywords: Diabetes, Diacylglycerol Acyltransferase-1, Particle Swarm Optimization, QSAR, Support Vector Machine