Human Oral Bioavailability dari Kandidat Obat Menggunakan Metode Simulated Annealing – Support Vector Machine

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Abstract

Pharmacokinetics is the science that studies the process by which drugs enter the body. HOB or human oral bioavailability is one of the important tests and references in drug manufacture. Limitations of human samples in experimental testing are obstacles to this process. In this study, we predicted HOB for drug candidates. This research was conducted using the dataset used in previous studies. The method used in this study uses Simulated Annealing as feature selection and the prediction method used is Support Vector Machine (SVM). This prediction process uses the three existing SVM kernels, namely, the Radial Basis Function (RBF) kernel, the Polynomial kernel, and the Linear kernel. The results show that the best SVM model is in the RBF kernel with an accuracy and F1-Score is 0.7968 and 0.7911

Key words: ***human oral bioavailability*****,** ***machine learning*****,** ***simulated annealing*****,** ***support vector machine***