Abstract—The environment, an essential component of life, is facing challengers from the growth of industry and the use chemicals, such as ionic liquids (ILs). Initially, ILs were considered environmentally friendly and useful in various fields, such as electrochemistry and catalysis, but some ILs are difficult to decompose and can pollute soil and water. ILs consist of organic cations and anions, each of which has advantages such as high thermal stability and low volatility. However, more ILs pollute the environment and inhibit the enzyme Acetylcholinesterase (AChE), causing damage to the ecosystem. In this study, we aimed to predict the toxicity of ionic liquids to enzyme acetylcholinesterase. AChE inhibition can be measured by colorimetry but can also be analyzed by in-silico and machine learning methods. One of the in-silico methods that will be used is support vector machine (SVM). This study was conducted to predict the toxicity of ionic liquids to AChE using SVM optimized by Firefly Algorithm. To optimize the model results, we used the Firefly Algorithm to select features with high correlation values. Furthermore, to improve the predictive accuracy of our model, hyperparameter tuning is applied to the RBF, polynomial, and linear kernels. Through this rigorous process, we aim to improve the model in accurately predicting the toxicity of ionic liquids to the active acetylcholinesterase enzyme based on the results. It was found that the SVM model with RBF kernel give the best results with the value of prediction with R^2_{train} 0.9291 and R^2_{test} 0.8339.

Keywords—*firefly algorithm, support vector machine, toxicity, fingerprint based.*