I. Introduction

The environment is an integral aspect of life on Earth, providing essential support for all living organisms. However, industrial and technological advancements, while beneficial in many ways, have also introduced significant environmental challenges, particularly due to the widespread use of chemicals in industrial processes [1]. Among these, ionic liquids (ILs) have emerged as a novel class of solvents with applications in diverse fields, including electrochemistry, catalysis, green chemistry, and as green solvents [1]. Initially celebrated as eco-friendly alternatives, ILs have come under scrutiny as some are derived from non-renewable energy sources and are challenging to degrade, potentially undermining their environmentally friendly reputation [2].

The release of ILs into the environment raises concerns about their toxicity. ILs can act as harmful pollutants, contributing to air pollution and adversely impacting both ecosystems and human health [3]. A notable effect of IL toxicity is the inhibition of the acetylcholinesterase enzyme (AChE), which plays a critical role in breaking down acetylcholine into acetate and choline [4], [5]. Disruption of AChE activity can lead to severe neurological issues, with documented cases of significant mortality in aquatic species, such as a 70.

Traditional methods for measuring AChE inhibition rely on colorimetric analysis, specifically using 5,5'-dithio-bis- (2-nitrobenzoic acid) (DTNB). This process involves monitoring the yellow color produced when choline reacts with DTNB, which reflects the degree of enzyme inhibition. However, this method is time-consuming, expensive, and not well-suited for large-scale applications [4]. As an alternative, in silico methods leveraging machine learning have gained traction for their efficiency and accuracy.

Several studies have explored the potential of in silico methods for predicting IL toxicity on AChE. In 2008, Torrecilla et al. compared Multiple Linear Regression (MLR) and Multilayer Perceptron (MLP) models, achieving prediction accuracies of 0.814 and 0.973, respectively, highlighting the superiority of the MLP model [7]. n 2012, Yan et al. enhanced MLR predictions to 0.877 using topological indices as features, demonstrating the importance of feature engineering [8]. Basant et al. (2015) utilized Convolutional Neural Networks (CNN) and Support Vector Machines (SVM), with CNN achieving a prediction accuracy of 0.922 and SVM 0.910 [9]. In 2019, Zhu et al. introduced the Extreme Learning Machine (ELM), which outperformed MLR with an accuracy of 0.964 compared to 0.917 [6].

Despite these advancements, there remains room for improvement, particularly through feature selection techniques. Feature selection is crucial for optimizing machine learning models by identifying the most relevant variables, thereby enhancing prediction accuracy and reducing computational complexity. The Firefly Algorithm (FA), inspired by the behavior of fireflies communicating through light signals, is a promising meta-heuristic optimization method for this purpose [10]. FA offers several advantages, including its ability to explore diverse solutions efficiently and its potential for rapid convergence to optimal solutions [10].

This study focuses on combining FA for feature selection with Support Vector Machine (SVM) for parameter optimization to predict the toxicity of ionic liquids on AChE. SVM is chosen for its robust performance in handling complex classification and regression problems, making it well-suited for predicting toxicity outcomes. By integrating FA and SVM, this research aims to achieve more accurate, efficient, and reliable predictions, contributing to the design of safer and more environmentally friendly chemical alternatives.