1. INTRODUCTION

The growing demand for clean and renewable energy, supported by stricter environmental regulations, has driven scientists to develop environmentally friendly chemical prod- ucts [1]. Ionic liquids (ILs) have garnered significant at- tention due to their low volatility, high thermal stability, and tunable physicochemical properties, making them ideal for applications like solvents, electrolytes, and catalysts [2]. However, extensive IL use raises environmental and health concerns, particularly regarding their toxicity to biological systems [3]. Studies suggest that ILs containing pyrindium and imidazolium inhibit enzyme activity, with acetylcholinesterase (AChE) inhibition in fish causing up to 70% mortality [4, 5]. Despite their antimicrobial benefits, ILs can harm vital uni- cellular organisms in ecosystems. Research has also shown that exposure to IL can alter microbial communities in soil and water, leading to reduced biodiversity and altered nutrient cycling [2].

AChE, an enzyme critical for nerve signal transmission, is commonly used to assess chemical toxicity due to its susceptibility to IL inhibition [5, 6, 7]. This enzyme breaks down acetylcholine into acetic acid and choline, and its inhibition poses neurotoxic risks [8]. Given the vast diversity of ILs—stemming from numerous cation and anion combi- nations—traditional toxicity testing methods are costly, labo- rious, and time-intensive [1, 10]. This highlights the need for in silico approaches to predict IL toxicity efficiently, with various computational models already developed for this purpose [1, 6]. Previous studies have explored IL toxicity prediction using different models. In 2008, Toreccilla achieved an R^2 of 0.973 using Multilayer Perceptron (MLP), while Yan et al. (2012) reached an R^2 of 0.877 with Multiple Linear Regression (MLR) and Topological Indexes [11, 12]. In 2015, Basant et al. reported an improved R^2 of 0.910 using Support Vector Machine (SVM) [9]. Further studies combining MLR and Extreme Learning Machine (ELM) with larger datasets also confirmed the superiority of non-linear models for IL toxicity prediction [1, 9]. However, these results could be enhanced through more advanced models like Artificial Neural Networks (ANNs).

Currently, ANN implementation often relies on manual parameter tuning, a time-consuming process that can yield inconsistent results [13]. To address this, auto-tuning methods such as metaheuristic algorithms have been introduced for architecture optimization [14]. One promising method is the Grey Wolf Optimizer (GWO), inspired by the hunting behavior of grey wolves, which offers efficient local search capabilities for parameter optimization [16].

This study focuses on predicting IL toxicity to AChE using an ANN optimized with GWO. The combination of ANN'sability to model complex, non-linear data and GWO's robust search mechanism is expected to enhance predictive accuracy
[15, 16].