Abstract

The aim of this study is to develop a predictive model to assess the toxicity of ionic liquids (ILs) towards acetyl-cholinesterase (AChE) enzymes, specifically evaluating the per- formance of the GWO-optimized ANN model in predicting ILs toxicity to AChE. An artificial neural network (ANN) optimised by the Grey Wolf Optimizer (GWO) was used. The excessive use of ILs, in spite of their low volatility and high thermal stability, raises concerns for the environment and human health due to their potential toxicity to biological systems. To address these issues, a dataset of 160 ILs was encoded using the PaDEL descriptor, and an ANN model was constructed and optimised using GWO to improve predictive performance. The optimised ANN model, configured with one hidden layer, 97 hidden nodes, a tanh activation function and the Adam optimiser, achieved a high prediction accuracy with an R^2 value of 0.870. These results demonstrate the effectiveness of the model in predicting IL toxicity and its potential to reduce reliance on traditional, labour-intensive toxicity assessment methods. Future research should explore the integration of more advanced metaheuristic algorithms to further improve model performance and extend its applicability to a wider range of chemical toxicity predictions. This approach has significant implications for the safer develop- ment of chemicals and environmental risk assessment.

Index Terms—acetylcholinesterase, artificial neural network, grey wolf algorithm, ioniq liquid, toxicity prediction.