Implementation of LSTM Tuned by Camel Algorithm for Predicting Toxicity of Ionic Liquids toward Acetylcholinesterase Enzymes

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Abstract

The environment is a major concern in the industry, including the use of solvents. One solvent that is widely used in the industrial field is ionic liquid. Some ionic liquids can pollute soil and aquatic ecosystems. This is due to the toxicity of ionic liquid which can inhibit the enzyme acetylcholinesterase. Therefore, the enzyme acetylcholinesterase can be used as an indicator of the toxicity of ionic liquid. In silico methods can be used to detect the toxicity of ionic liquids. This study proposes a LSTM model optimized by the Camel algorithm to predict the toxicity of ionic liquids toward AChE enzymes. The model uses a dataset of 160 ionic liquids, encoded via SMILES-to-vector. The optimization scheme is a combination of the parameters in the camel algorithm, such as population size, burden factor, supply init, and death rate with a maximum of 25 iterations. Based on the results, we found that the best model is LSTM with 126 embedding nodes, 3 layers LSTM with 134, 71, and 53 nodes, and 0.2 dropouts with the value of R2 score 0.747 on testing sets. LSTM model effectively captured the sequential patterns in SMILES and improved the toxicity prediction of ionic liquids toward the acetylcholinesterase enzyme.

Keywords: ionic liquid, toxicity, acetylcholinesterase enzyme, long short-term memory, optimization, camel algorithm.