Abstract

Blood-Brain Barrier Penetration (BBBp) is the capability of a substance or chemical compound to cross the blood-brain barrier (BBB), a natural protective system between the bloodstream and brain tissue that restricts and controls what can enter the brain. With an estimated 98% of small molecules unable to cross the BBB, reliable and efficient computational methods are urgently needed to predict BBB penetration. Detection of Blood-Brain Barrier Penetration can be conducted using techniques such as NeuroCart. Physicochemical properties can be utilized as molecular features to predict BBBp, and in silico BBBp models can enhance uncertainty estimation techniques. However, formal meta-analysis cannot be performed due to the large number of tests and variations in their implementation. Therefore, methods that can reliably predict BBB penetration from drug candidates are urgently needed. This study aims to implement Firefly Algorithm-Support Vector Machine in predicting Blood-Brain Barrier Penetration of drug candidate. There are several kernels used such as linear kernel, polynomial kernel, and Radial Basic Function (RBF) kernel. The three kernels get different results or performance, and The Radial Basic Function (RBF) kernel shows strong performance with testing accuracy of 0.870 and F1 value of 0.920. These results underscore the potential of polynomial and RBF kernels for wider applications in predictive modeling tasks

Keywords : Blood-Brain Barrier Penetration (BBBp), Blood-Brain Barrier (BBB), Firefly Algorithm (FA), Support Vector Machine (SVM), Feature Selection, Machine Learning, Predictive Modeling