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Machine Learning Approach In Solubility Enhancement Of Dextromethorphan Syrup Using Molecular Descriptor

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ABSTRACT

Dextromethorphan is a commonly prescribed antitussive agent; however, its therapeutic effectiveness can be limited by physicochemical constraints such as moderate aqueous solubility and inconsistent dissolution behaviour. Enhancing its solubility is therefore essential to improve bioavailability and formulation performance. The present study focuses on improving the solubility profile of dextromethorphan using a molecular descriptor based computational approach integrated with Machine Learning (ML) tools. A comprehensive set of molecular descriptors—including topological indices, hydrogen bond donor and acceptor counts, logP, polar surface area, molecular flexibility, and relevant electronic parameters were generated to characterize the molecule. These descriptors served as input variables for building predictive ML models. An Artificial Neural Network (ANN) model was developed to establish quantitative relationships between molecular features and solubility outcomes. The optimized ANN model demonstrated high predictive performance and successfully identified critical structural attributes influencing solubility enhancement. This ML-guided strategy minimized the need for extensive experimental screening and facilitated rational, targeted formulation development aimed at improving aqueous solubility and dissolution rate. Overall, the study underscores the potential of data-driven molecular modelling and artificial intelligence tools in modern pharmaceutical formulation design and offers a scalable approach for addressing solubility challenges of poorly water-soluble drugs.

Keywords - Dextromethorphan, Solubility Enhancement, Molecular Descriptors, Artificial Neural Network, Machine Learning.