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PREDICTING INTESTINAL PERMEATION OF DRUGS THROUGH NEURAL NETWORK ANALYSIS BASED ON SOME MOLECULAR DESCRIPTORS

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Utilization of a neural network model was used as computer algorithm to predict intestinal absorption of drugs based on various molecular properties. In the search for new drugs, a major problem encountered is obtaining drug structures which, as well as being potent in vitro, possess favourable pharmacokinetic profiles which enable them to pass easily through the relevant body membranes, especially the gastrointestinal epithelia, to effect their action. Since most drugs are mostly absorbed passively, this work aimed at simplifying and improving the prediction of intestinal drug absorption through a generated model. The model was generated by neural network analysis of some molecular descriptors, obtained via molecular modelling, corresponding to the empirically determined caco-2 cell permeability coefficient of the molecule. Utilization of a neural network model is good way to find a nonlinear relationship between causal factors and their results. Most of the parameters were based on polar surface area (PSA) for predicting Caco-2 cell permeability and human intestinal absorption.

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