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Antibacterial Evaluation, in Silico ADME and QSAR Studies of Some Benzimidazole Derivatives

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Abstract : In this paper, various derivatives of benzimidazole have been evaluated against Gram-negative bacteria Escherichia coli. For all investigated compounds the minimum inhibitory concentration (MIC) was determined. Quantitative structure-activity relationships (QSAR) attempts to find consistent relationships between the variations in the values of molecular properties and the biological activity for a series of compounds so that these rules can be used to evaluate new chemical entities. The correlation between MIC and some absorption, distribution, metabolism and excretion (ADME) parameters was investigated, and the mathematical models for predicting the antibacterial activity of this class of compounds were developed. The quality of the multiple linear regression (MLR) models was validated by the leave-one-out (LOO) technique, as well as by the calculation of the statistical parameters for the developed models and the results are discussed on the basis of the statistical data. The results of this study indicate that ADME parameters have a significant effect on the antibacterial activity of this class of compounds. Principal component analysis (PCA) and agglomerative hierarchical clustering algorithms (HCA) confirmed that the investigated molecules can be classified into groups on the basis of the ADME parameters: Madin-Darby Canine Kidney cell permeability (MDCK), Plasma protein binding (PPB%), human intestinal absorption (HIA%) and human colon carcinoma cell permeability (Caco-2).

Keywords : benzimidazoles, QSAR, ADME, in silico
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