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Chemometric Estimation of Inhibitory Activity of Benzimidazole Derivatives by Linear Least Squares and Artificial Neural Networks Modelling

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Abstract : The subject of this paper is to correlate antibacterial behavior of benzimidazole derivatives with their molecular characteristics using chemometric QSAR (Quantitative Structure–Activity Relationships) approach. QSAR analysis has been carried out on the inhibitory activity of benzimidazole derivatives against Staphylococcus aureus. The data were processed by linear least squares (LLS) and artificial neural network (ANN) procedures. The LLS mathematical models have been developed as a calibration models for prediction of the inhibitory activity. The quality of the models was validated by leave one out (LOO) technique and by using external data set. High agreement between experimental and predicted inhibitory acivities indicated the good quality of the derived models. These results are part of the CMST COST Action No. CM1306 "Understanding Movement and Mechanism in Molecular Machines".

Keywords : Antibacterial, benzimidazoles, chemometric, QSAR.
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