World Academy of Science, Engineering and Technology
International Journal of Bioengineering and Life Sciences
Vol:9, No:07, 2015

Quantitative Structure–Activity Relationship Analysis of Some Benzimidazole Derivatives by Linear Multivariate Method

Authors : Strahinja Z. Kovačević, Lidija R. Jevrić, Sanja O. Podunavac Kuzmanović

Abstract : The relationship between antibacterial activity of eighteen different substituted benzimidazole derivatives and their molecular characteristics was studied using chemometric QSAR (Quantitative Structure–Activity Relationships) approach. QSAR analysis has been carried out on inhibitory activity towards Staphylococcus aureus, by using molecular descriptors, as well as minimal inhibitory activity (MIC). Molecular descriptors were calculated from the optimized structures. Principal component analysis (PCA) followed by hierarchical cluster analysis (HCA) and multiple linear regression (MLR) was performed in order to select molecular descriptors that best describe the antibacterial behavior of the compounds investigated, and to determine the similarities between molecules. The HCA grouped the molecules in separated clusters which have the similar inhibitory activity. PCA showed very similar classification of molecules as the HCA, and displayed which descriptors contribute to that classification. MLR equations, that represent MIC as a function of the in silico molecular descriptors were established. The statistical significance of the estimated models was confirmed by standard statistical measures and cross-validation parameters (SD = 0.0816, F = 46.27, R = 0.9791, R2CV = 0.8266, R2adj = 0.9379, PRESS = 0.1116). These parameters indicate the possibility of application of the established chemometric models in prediction of the antibacterial behaviour of studied derivatives and structurally very similar compounds.

Keywords : antibacterial, benzimidazole, molecular descriptors, QSAR
Conference Title : ICBBBE 2015 : International Conference on Biochemical, Biomolecular and Biopharmaceutical Engineering
Conference Location : Stockholm, Sweden
Conference Dates : July 13-14, 2015