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Quantitative Structure-Property Relationship Study of Base Dissociation Constants of Some Benzimidazoles

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Abstract : Benzimidazoles are a group of compounds with significant antibacterial, antifungal and anticancer activity. The studied compounds consist of the main benzimidazole structure with different combinations of substituens. This study is based on the two-dimensional and three-dimensional molecular modeling and calculation of molecular descriptors (physicochemical and lipophilicity descriptors) of structurally diverse benzimidazoles. Molecular modeling was carried out by using ChemBio3D Ultra version 14.0 software. The obtained 3D models were subjected to energy minimization using molecular mechanics force field method (MM2). The cutoff for structure optimization was set at a gradient of 0.1 kcal/Åmol. The obtained set of molecular descriptors was used in principal component analysis (PCA) of possible similarities and dissimilarities among the studied derivatives. After the molecular modeling, the quantitative structure-property relationship (QSPR) analysis was applied in order to get the mathematical models which can be used in prediction of pKb values of structurally similar benzimidazoles. The obtained models are based on statistically valid multiple linear regression (MLR) equations. The calculated cross-validation parameters indicate the high prediction ability of the established QSPR models. This study is financially supported by COST action CM1306 and the project No. 114-451-347/2015-02, financially supported by the Provincial Secretariat for Science and Technological Development of Vojvodina.

Keywords : benzimidazoles, chemometrics, molecular modeling, molecular descriptors, QSPR
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