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Synthesis, biological evaluation and 3D QSAR of some novel benzimidazole derivatives as anti-microbial compounds

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Benzimidazoles are an important group of heterocyclic compounds that are biologically active and of significant importance in medicinal chemistry. In light of affinity they display towards a variety of enzymes and protein receptors, medicinal chemists should certainly classify them as privileged 'substructures' for drug dosing. The incorporation of the nucleus is an important synthetic strategy in studies of antimicrobial drug discovery. In the past few decades, benzimidazole and its derivatives have received much attention due to their chemotherapeutic values. We have synthesized *p*-substituted acetanilide, *p*-substituted nitro acetanilide, *p*-substituted nitro aniline, *p*-substituted phenylenediamine. There after substituted mercaptobenzimidazoles and thio-methyl-pyridine substituted benzimidazoles were synthesized from these were synthesized by cyclization and condensation reactions. All these newly synthesized derivatives were confirmed by IR, H-NMR and mass spectra. Antimicrobial study of these compounds against Gram +ve and Gram -vemicro organisms and using ciprofloxacin as standard.Someof the compounds showed moderate activity. With an objective to generate computational model, which can be used to design new derivatives in the series using the data accumulated by the current study, it wasintended to do a computational 3D-QSAR studies. The models generated by TopomerCoMFA were in the form of contour plots which showed the requirement of steric and electrostatic fields in the different regions of the fragments formed during the study with an $r^2$of 0.725-0.843 and q^2 of 0.610-0.636. All the models generated, demonstrated goodpredictivity which suggests that our approaches may be beneficial for discovery of novel molecules on the path of rational drug discovery which can ultimately save time, money and efforts at wet lab end.

Biography

SonalDubeyhas completed PhD in 2003. Since then she is actively involved in academics and research. She is presently working as Professor and HOD of Dept. of Pharm. Chemistry, at Krupanidhi College of Pharmacy. She has published one book, more than 30 papers in reputed journals and has been serving as an editorial board member of repute.

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