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Synthesis, anti-bacterial and molecular docking studies of new benzimidazole derivatives

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The organic compounds particularly with heterocyclic ring system promote wide range of activities via effective binding to enzyme receptor site. Several thousands of new heterocyclic compounds, either synthesized in the laboratories or isolated from natural sources are added to the literature every year. Many of these compounds have drawn the attention of research scientists on the basis of their therapeutic, biological and industrial potential. In the present study, various benzimidazole fused triazinane 4-thione heterocyclic moieties are synthesized by cyclic condensation based on classical Mannich amino methylation of N,N' unsymmetrical thio ureas with 30% HCHO and methyl amine in ethanol. The condensation reaction between a methyl amine and formaldehyde yields an aliphatic imine. The imine is unstable and immediately cyclizes to yield the correspond 1,3,5-triazinane. From the stand point of biological activity, fused heterocyclic systems like benzimidazole and triazinane derivatives are often of much greater interest than the constituent cyclic compounds. All the newly synthesized compounds 3 (a-e) and 4 (a-e) were screened for their antibacterial activity against *Bacillus subtilis, Bacillus cereus, Staphylococcus aureus, E. coli, Klebsielia pneumonia, and Salmonella* Typhi. Some of the compounds have excellent antibacterial activity against the test bacteria and nearly equal to the standard drug. Remaining compounds showed moderate to least activity or no activity. The results of molecular docking studies showed good agreement with the *in vivo* analysis all ten compounds were docked into the active sites of both proteins, i.e., *S. aureus* tyrosyl tRNA synthetase and *E. coli* topoisomerase II DNA Gyrase B. Few of the compounds showed good free energy of binding and inhibition constant with both proteins. The structures of newly synthesized and characterized by melting points, TLC, compounds have been established by elemental analysis and spectral data (IR, NMR & Mass) were screened for antimicrobial and docking studies some of them compounds showed promising activity against the test organisms employed.

Biography

G Brahmeshwari has completed her PhD in 1995 from Kakatiya University; Warangal (AP) India. She has more than 20 years of academic experience in teaching at various institutions. Currently she is working as an Assistant Professor of Chemistry in Arts and Science College, Kakatiya University and she served as Joint Director of Padmakshi Women's Hostel K.U and In-charge Department of Chemistry in Arts & Science College Kakatiya University and also organized workshop for UG courses on revised syllabus. She is acting Deputy Director of Science Courses SDLCE and Member of Board of Studies for UG. She has been in the research field by admitting five Research scholars under her supervision since November 2011. She has published 9 papers in reputed journals.

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