

MERCAPTOIMIDAZOLES AS A NOVEL CLASS OF ANTIMICROBIAL AGENTS: GREEN SYNTHESIS AND COMPUTATIONAL STUDIES

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In search of a new class of potential antimicrobial agents, some 1,4-diary 1-2-mercaptoimidazoles were prepared by employing greener synthetic approach in which substituted anilines were treated with phenacyl bromide in the presence of $\text{Na}_2\text{CO}_3/\text{K}_2\text{CO}_3$ followed by the treatment of a solid catalyst, *p*-TSA. All compounds were characterized on the basis of their spectral data. Pharmacotherapeutic potential of the compounds was estimated on the basis of prediction of activity spectra for substances (PASS) and prediction results were obtained by Pharma Expert software. The activity profile predicted by PASS was further supported by some theoretical calculations, *in vitro* experimental evaluation and then validated via docking studies. On the basis of all experimentation, it is concluded that the compounds considered under this investigation have an excellent potential to be acted as antimicrobial leads in the future.

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