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SYNTHESIS, BIOLOGICAL SCREENING AND DFT STUDIES OF THE NEW TETRAHYDROPYRIMIDINE-BENZO[D]IMIDAZOL COMPOUNDS

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A series of the tetrahydropyrimidines obtained through the Biginelli condensation was used to synthesize new tetrahydropyrimidine-benzo[d]imidazoles, by two types of reactions: Mannich reaction or reaction with a benzimidazole halogen compound. The structures of all compounds were confirmed by ^{1}H, ^{13}C-NMR, FTIR, UV-VIS spectra and elemental analysis. All derivatives were evaluated by qualitative and quantitative methods against a panel of selected bacterial and fungal strains. A DFT analysis of molecular structure and frontier molecular orbitals HOMO-LUMO was performed using the GAMESS 2012 software. Antimicrobial activity was correlated with electronic parameters (chemical hardness, electronic chemical potential, global electrophilicity index), Mullikan atomic charges and geometric parameters of the tetrahydropyrimidines calculated with GAMESS. It has been found that the symmetry of the molecule and the presence of nucleophilic group are advantages for a high antimicrobial activity.

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